



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:26 PM UTC

PDB ID : 9S78 / pdb_00009s78
Title : Yeast 20S Proteasome in Complex with Tellurophene-Tagged Carfilzomib
Authors : Potter, N.; Eddenden, A.; Fomina, A.; Dinesh, A.; Jackson, H.W.; McGuigan, A.; Groll, M.; Nitz, M.
Deposited on : 2025-08-04
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

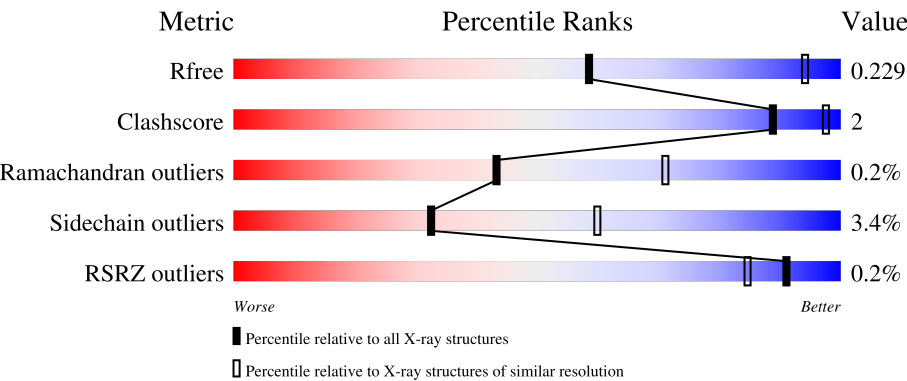
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



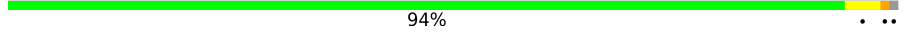
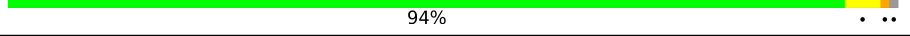
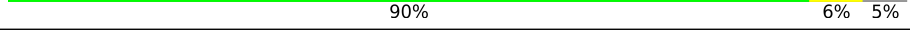
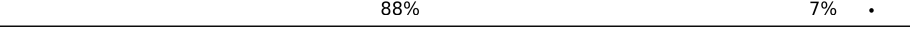
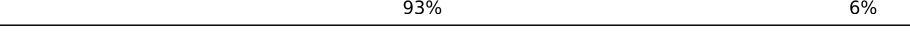
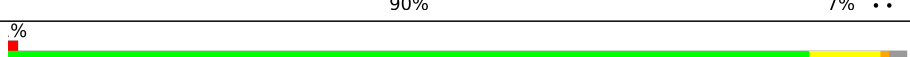
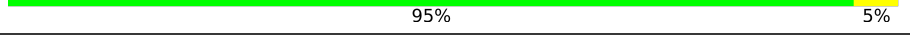
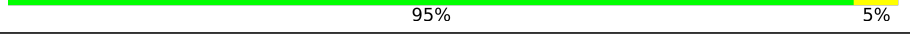
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	97%
1	O	250	96%
2	B	258	90% 5%
2	P	258	90% 5%
3	C	254	88% 6% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	e	5	
15	f	5	

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Mol	Chain	Length	Quality of chain
15	g	5	
15	h	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	00E	h	1	-	-	X	-
16	MG	I	301	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49638 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	240	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Carfilzomib (Tellurophene-Tagged).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	Te	0	0	0
			58	42	6	9	1			
15	f	5	Total	C	N	O	Te	0	0	0
			58	42	6	9	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	g	5	Total	C	N	O	Te	0	0	0
			58	42	6	9	1			
15	h	5	Total	C	N	O	Te	0	0	0
			58	42	6	9	1			

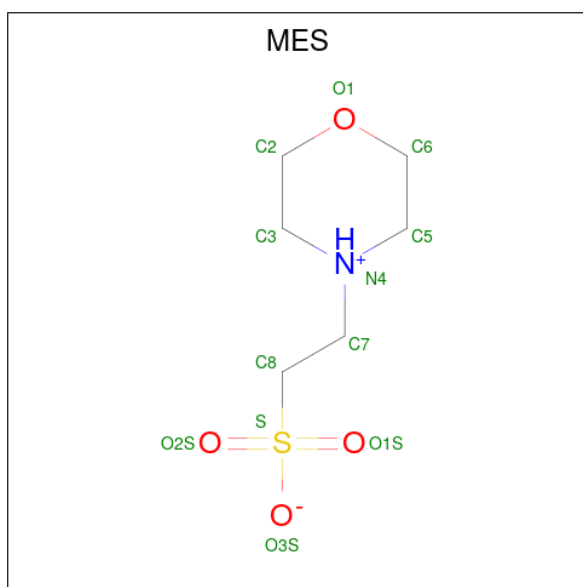
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		
17	b	1	Total	Cl	0	0
			1	1		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	f	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	h	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	3	Total	O	0	0
			3	3		
19	B	3	Total	O	0	0
			3	3		
19	C	3	Total	O	0	0
			3	3		
19	E	1	Total	O	0	0
			1	1		
19	F	2	Total	O	0	0
			2	2		
19	G	2	Total	O	0	0
			2	2		
19	H	2	Total	O	0	0
			2	2		
19	I	3	Total	O	0	0
			3	3		

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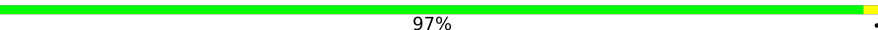
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	J	8	Total O 8 8	0	0
19	K	4	Total O 4 4	0	0
19	L	4	Total O 4 4	0	0
19	M	6	Total O 6 6	0	0
19	N	4	Total O 4 4	0	0
19	P	3	Total O 3 3	0	0
19	Q	2	Total O 2 2	0	0
19	T	2	Total O 2 2	0	0
19	U	6	Total O 6 6	0	0
19	V	2	Total O 2 2	0	0
19	W	1	Total O 1 1	0	0
19	X	6	Total O 6 6	0	0
19	Y	2	Total O 2 2	0	0
19	Z	4	Total O 4 4	0	0
19	a	3	Total O 3 3	0	0
19	b	6	Total O 6 6	0	0
19	h	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

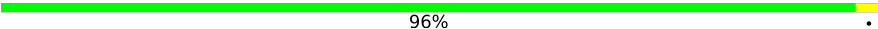
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proteasome subunit alpha type-2

Chain A:  97%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96%



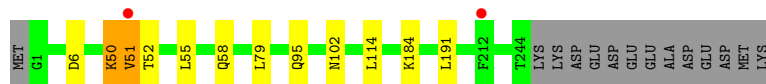
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  90% 5%



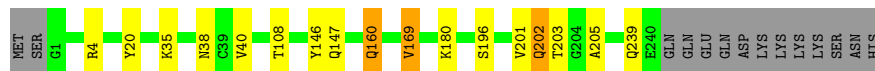
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  90% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  88% 6% 6%



- Molecule 3: Proteasome subunit alpha type-4

MTT	SR	R4	N38	L50	T108	Q116	T119	Y146	Q147	Q160	V169	K180	G189	S196	V201	Q202	T203	G204	A205	Q239	E240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729
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MET	PHE	LEU	THR	ARG	SER	GLU	TYR	D1	R2	G3	G4	S5	T6	L20	L40	V60	I99	E117	GLY	ALA	SER	GLY	GLU	GLU	ARG	L125	N160	L176	W179	L193	K197	I214	K236	E242	SER	PRO	GLU	GLU	GLU	ALA	ASP	ASP	VAL	GLU	MET
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MET	PHE	LEU	THR	ARG	SER	GLU	TYR	D1	R2	G2	G3	V4	S5	L20	L40	V60	I99	F115	G116	E117	GLY	ALA	SER	GLY	GLU	GLU	ARG	L125	N160	L176	W179	L193	K197	I214	K236	E242	S249	PRO	GLU	GLU	ASP	VAL	GLU	MET
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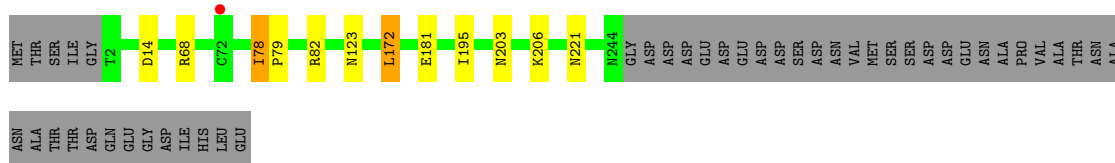
Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows the amino acid sequence: MET, PHE, ARG, N3, T9, L25, K29, E54, L71, A77, P78, L87, A107, T119, L188, and I233. MET, PHE, and ARG are in grey boxes, indicating they are not part of the motif. N3, T9, L25, K29, E54, L71, A77, P78, L87, A107, T119, L188, and I233 are in yellow boxes, indicating they are part of the motif. The height of each bar indicates its relative frequency at that position.

Position	Type	Count (approx.)
MET	Grey	1
PHE	Yellow	1
ARG	Grey	1
N3	Green	1
T9	Orange	1
L25	Yellow	4
K29	Yellow	3
E54	Yellow	2
L71	Orange	4
A77	Yellow	3
P78	Yellow	2
L87	Yellow	2
A107	Yellow	2
C112	Yellow	2
T119	Yellow	1
L188	Yellow	2
I233	Green	2

MET	THR	SER	ILE	GLY	T2	D14	R68	I78	P79	N123	L172	E181	I195	N203	K206	C215	N221	N244	GLY	ASP	ASP	ASP	ASP	GLU	GLU	GLU	ASP	ASP	SER	ASP	ASP	ASN	VAL	MET	SER	SER	ASP	ASP	GLU	GLU	ASN	ALA	ALA	VAL	THR	ALA	ALA	ASN
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THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 90% 5% .



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 6% 5%



- Molecule 8: Proteasome subunit beta type-2

Chain H: 90% 6% .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 88% 7% .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 93% 6%

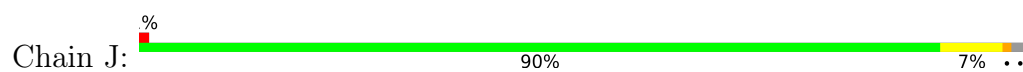


- Molecule 9: Proteasome subunit beta type-3

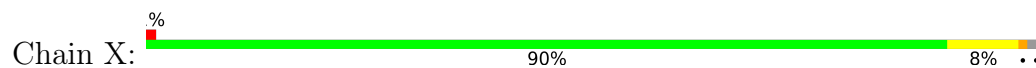
Chain W: 91% 8%



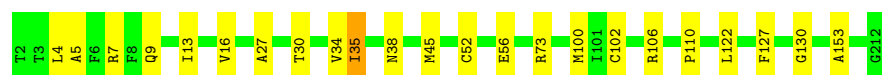
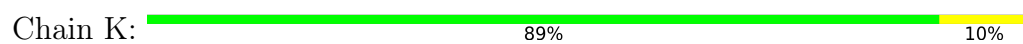
- Molecule 10: Proteasome subunit beta type-4



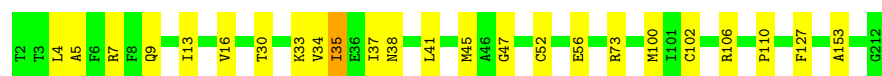
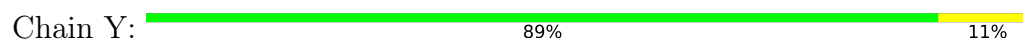
- Molecule 10: Proteasome subunit beta type-4



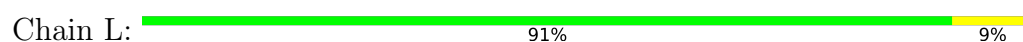
- Molecule 11: Proteasome subunit beta type-5



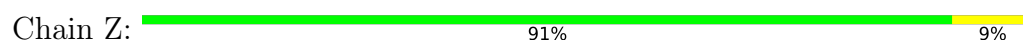
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7

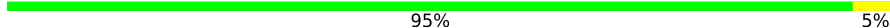


- Molecule 13: Proteasome subunit beta type-7

Chain a:  88% 7% 5%

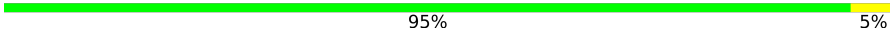


- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% 5%

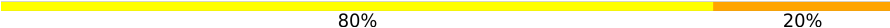


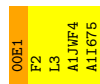
- Molecule 14: Proteasome subunit beta type-1

Chain b:  95% 5%



- Molecule 15: Carfilzomib (Tellurophene-Tagged)

Chain e:  80% 20%

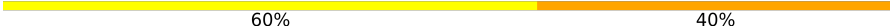


- Molecule 15: Carfilzomib (Tellurophene-Tagged)

Chain f:  80% 20%



- Molecule 15: Carfilzomib (Tellurophene-Tagged)

Chain g:  60% 40%



- Molecule 15: Carfilzomib (Tellurophene-Tagged)

Chain h:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.64Å 300.25Å 144.75Å 90.00° 113.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 30.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-3.15) 96.7 (30.00-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.223 0.196 , 0.229	Depositor DCC
R_{free} test set	8857 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49638	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, HPE, A1I67, MG, CL, A1JWF, 00E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	0/1952	1.44	0/2642
1	O	1.04	0/1952	1.44	0/2642
2	B	1.03	0/1934	1.46	0/2618
2	P	1.03	0/1934	1.45	0/2618
3	C	1.03	0/1910	1.48	0/2586
3	Q	1.03	0/1910	1.48	0/2586
4	D	1.04	0/1837	1.47	0/2475
4	R	1.03	0/1837	1.47	0/2475
5	E	1.03	0/1800	1.45	0/2433
5	S	1.03	0/1800	1.45	0/2433
6	F	1.02	0/1932	1.45	0/2609
6	T	1.02	0/1932	1.45	0/2609
7	G	1.02	0/1945	1.44	0/2634
7	U	1.02	0/1941	1.45	0/2629
8	H	1.05	0/1708	1.44	0/2316
8	V	1.05	0/1708	1.45	0/2316
9	I	1.01	0/1611	1.42	0/2174
9	W	1.02	0/1611	1.42	0/2174
10	J	1.01	0/1589	1.42	0/2142
10	X	1.01	0/1589	1.43	0/2142
11	K	1.01	0/1674	1.43	0/2264
11	Y	1.01	0/1674	1.44	0/2264
12	L	1.00	0/1795	1.39	0/2420
12	Z	1.00	0/1795	1.39	0/2420
13	M	1.02	0/1855	1.40	0/2514
13	a	1.02	0/1855	1.40	0/2514
14	N	1.02	0/1541	1.47	0/2087
14	b	1.02	0/1541	1.46	0/2087
15	e	1.52	0/7	1.72	0/8
15	f	1.49	0/7	1.71	0/8
15	g	1.23	0/7	1.41	0/8
15	h	1.33	0/7	1.73	0/8

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.02	0/50190	1.44	0/67855

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	f	0	1
15	h	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	f	4	A1JWF	Peptide
15	h	4	A1JWF	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1903	0	1898	6	0
8	H	1677	0	1678	6	0
8	V	1677	0	1678	9	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	10	0
11	K	1637	0	1585	15	0
11	Y	1637	0	1585	20	0
12	L	1757	0	1711	8	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	6	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	4	0
15	e	58	0	31	8	0
15	f	58	0	31	9	0
15	g	58	0	31	9	0
15	h	58	0	31	19	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	H	12	0	13	0	0
18	V	12	0	13	1	0
18	f	12	0	13	0	0
18	h	12	0	13	1	0
19	A	3	0	0	0	0
19	B	3	0	0	0	0
19	C	3	0	0	0	0
19	E	1	0	0	0	0
19	F	2	0	0	0	0
19	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	2	0	0	0	0
19	I	3	0	0	0	0
19	J	8	0	0	0	0
19	K	4	0	0	0	0
19	L	4	0	0	0	0
19	M	6	0	0	0	0
19	N	4	0	0	0	0
19	P	3	0	0	0	0
19	Q	2	0	0	0	0
19	T	2	0	0	0	0
19	U	6	0	0	0	0
19	V	2	0	0	0	0
19	W	1	0	0	0	0
19	X	6	0	0	0	0
19	Y	2	0	0	0	0
19	Z	4	0	0	0	0
19	a	3	0	0	0	0
19	b	6	0	0	0	0
19	h	1	0	0	0	0
All	All	49638	0	49201	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:108:HIS:HE1	15:h:1:00E:HE1	1.09	1.12
12:Z:108:HIS:CE1	15:h:1:00E:HE1	1.89	1.06
11:Y:33:LYS:NZ	15:h:5:A1I67:CG2	2.24	1.01
12:L:108:HIS:CE1	15:f:1:00E:HE2	2.10	0.86
11:Y:33:LYS:HZ3	15:h:5:A1I67:CG2	1.87	0.84
9:I:124:ASP:HB3	15:e:3:LEU:CD1	2.07	0.84
9:W:124:ASP:HB3	15:g:3:LEU:CD1	2.09	0.81
9:W:124:ASP:HB3	15:g:3:LEU:HD12	1.63	0.79
11:Y:33:LYS:HZ2	15:h:5:A1I67:CG2	1.94	0.77
12:L:108:HIS:HE1	15:f:1:00E:HE2	1.49	0.77
15:e:3:LEU:HD12	15:e:3:LEU:N	2.01	0.75
15:h:3:LEU:N	15:h:3:LEU:HD23	2.03	0.74
11:Y:4:LEU:HD12	11:Y:4:LEU:C	2.14	0.72
11:K:4:LEU:C	11:K:4:LEU:HD12	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:108:HIS:CE1	15:h:1:00E:CE1	2.71	0.70
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.73	0.70
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.68
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.75	0.68
11:Y:4:LEU:HD12	11:Y:4:LEU:O	1.94	0.68
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.75	0.68
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.76	0.67
15:e:3:LEU:HD12	15:e:3:LEU:H	1.59	0.65
14:b:152:VAL:HA	14:b:175:MET:HE1	1.78	0.65
14:N:152:VAL:HA	14:N:175:MET:HE1	1.79	0.63
12:Z:108:HIS:NE2	15:h:1:00E:CD1	2.64	0.60
14:N:7:THR:HG23	14:N:123:PRO:O	2.01	0.60
8:V:46:ALA:HB2	15:g:5:A1I67:CG2	2.32	0.60
11:Y:33:LYS:HD3	15:h:5:A1I67:CG2	2.32	0.59
10:J:174:MET:HA	10:X:174:MET:HA	1.83	0.59
12:Z:108:HIS:NE2	15:h:1:00E:HD1	2.18	0.59
15:h:1:00E:HD1	15:h:1:00E:O	2.02	0.59
14:b:7:THR:HG23	14:b:123:PRO:O	2.03	0.58
15:f:1:00E:O	15:f:1:00E:HD2A	2.03	0.58
8:H:4:VAL:HG12	8:H:126:SER:CB	2.34	0.58
15:e:1:00E:O	15:e:1:00E:HD1A	2.04	0.57
6:F:78:ILE:HB	6:F:79:PRO:HD3	1.87	0.56
8:V:42:TRP:CG	8:V:176:CYS:HG	2.24	0.56
9:W:177:ASP:OD2	9:W:180:SER:OG	2.23	0.55
9:I:177:ASP:OD2	9:I:180:SER:OG	2.23	0.55
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.89	0.55
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.43	0.54
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.89	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
15:f:5:A1I67:C59	15:f:5:A1I67:N	2.72	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.52
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.43	0.52
6:T:78:ILE:HB	6:T:79:PRO:HD3	1.91	0.52
8:V:46:ALA:CB	15:g:5:A1I67:CG2	2.88	0.52
8:V:210:THR:HG21	9:W:167:SER:HB3	1.91	0.52
15:g:1:00E:O	15:g:1:00E:HD2	2.09	0.52
11:K:27:ALA:CB	15:f:3:LEU:HD22	2.39	0.52
18:V:302:MES:O1S	15:g:5:A1I67:O60	2.27	0.51
15:g:5:A1I67:N	15:g:5:A1I67:C59	2.73	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.50
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.44	0.50
7:G:78:ILE:N	7:G:79:PRO:CD	2.75	0.49
15:h:4:A1JWF:C	15:h:5:A1I67:C59	2.90	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
8:H:210:THR:HG21	9:I:167:SER:HB3	1.94	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.49
11:Y:4:LEU:C	11:Y:4:LEU:CD1	2.85	0.49
12:Z:108:HIS:HE1	15:h:1:00E:CE1	2.00	0.49
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.95	0.49
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.95	0.48
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.95	0.48
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.48
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.95	0.48
12:Z:108:HIS:CE1	15:h:1:00E:CD1	2.95	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.95	0.48
11:K:7:ARG:NH1	11:K:110:PRO:O	2.46	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.48
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.95	0.48
9:I:124:ASP:HB3	15:e:3:LEU:HD13	1.93	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.48
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.96	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.29	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.50	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.97	0.47
9:I:124:ASP:HB3	15:e:3:LEU:HD12	1.92	0.47
15:h:2:HPE:HB2	15:h:2:HPE:HE2	1.63	0.47
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.97	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
11:Y:33:LYS:CD	15:h:5:A1I67:CG2	2.93	0.46
15:f:4:A1JWF:C	15:f:5:A1I67:C59	2.93	0.46
12:L:147:MET:N	12:L:148:PRO:HD2	2.29	0.46
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.30	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
11:K:5:ALA:HB3	11:K:100:MET:CE	2.45	0.46
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.44	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:47:GLY:O	15:h:5:A1I67:N	2.49	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.44	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.30	0.46
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.45	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.16	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.97	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.45
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.16	0.45
11:Y:30:THR:OG1	12:Z:132:GLU:OE2	2.35	0.45
3:Q:116:GLN:O	3:Q:119:THR:OG1	2.34	0.45
4:R:4:VAL:CG1	4:R:115:PHE:CD2	3.00	0.45
15:f:3:LEU:H	15:f:3:LEU:HG	1.55	0.45
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.99	0.45
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.99	0.44
5:E:77:ALA:N	5:E:78:PRO:CD	2.81	0.44
8:V:2:THR:OG1	8:V:169:SER:OG	2.27	0.44
15:e:3:LEU:CD1	15:e:3:LEU:N	2.73	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.44
4:D:2:ARG:HD2	4:D:6:THR:HG21	1.98	0.44
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.00	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.44
8:H:4:VAL:HG12	8:H:126:SER:HB3	2.00	0.44
14:N:133:PHE:HA	14:b:132:THR:O	2.18	0.44
11:K:30:THR:OG1	12:L:132:GLU:OE2	2.34	0.43
13:M:220:ASP:O	13:M:223:LYS:HG2	2.18	0.43
10:X:168:LEU:O	10:X:172:MET:HB2	2.17	0.43
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.99	0.43
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.00	0.43
10:J:168:LEU:O	10:J:172:MET:HB2	2.18	0.43
15:f:2:HPE:HB2	15:f:2:HPE:HE2	1.59	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.00	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.99	0.43
13:a:220:ASP:O	13:a:223:LYS:HG2	2.18	0.43
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.54	0.43
4:R:4:VAL:HG11	4:R:115:PHE:HD2	1.84	0.43
7:G:34:LEU:C	7:G:34:LEU:HD23	2.44	0.42
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.02	0.42
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:13:ILE:HG13	11:Y:153:ALA:HB1	2.01	0.42
11:K:13:ILE:HG13	11:K:153:ALA:HB1	2.01	0.42
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.01	0.42
15:h:5:A1I67:O48	18:h:101:MES:O3S	2.38	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.68	0.42
5:S:112:CYS:SG	6:T:82:ARG:HD3	2.59	0.42
11:K:38:ASN:OD1	11:K:38:ASN:C	2.62	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.62	0.42
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.02	0.41
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.50	0.41
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.50	0.41
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
8:V:34:LEU:HD12	8:V:34:LEU:HA	1.92	0.41
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.02	0.41
11:K:4:LEU:HD12	11:K:4:LEU:O	2.20	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.03	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
3:C:35:LYS:HA	3:C:40:VAL:HA	2.03	0.41
3:C:201:VAL:O	3:C:202:GLN:CB	2.68	0.41
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.55	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.02	0.41
1:O:119:GLN:O	1:O:122:THR:HB	2.20	0.41
15:h:2:HPE:O	15:h:2:HPE:HG3	2.19	0.41
10:J:173:PRO:HB3	10:X:22:THR:HG21	2.02	0.41
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.55	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.41
5:S:71:LEU:C	5:S:71:LEU:CD2	2.94	0.41
7:U:34:LEU:HD23	7:U:34:LEU:C	2.45	0.41
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.03	0.41
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.03	0.41
11:K:130:GLY:HA3	15:f:5:A1I67:O	2.21	0.41
9:W:4:SER:CB	15:g:1:00E:HE1A	2.51	0.41
5:E:71:LEU:CD2	5:E:71:LEU:C	2.94	0.41
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	2.02	0.41
1:O:55:LEU:HB3	7:U:159:ALA:O	2.21	0.41
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.02	0.41
10:J:169:GLU:O	10:X:177:LYS:NZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:5:ALA:HB3	11:K:100:MET:HE2	2.03	0.40
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.40
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	2.03	0.40
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.04	0.40
15:e:3:LEU:CD1	15:e:3:LEU:H	2.31	0.40
8:H:3:ILE:O	8:H:3:ILE:HG13	2.22	0.40
4:R:4:VAL:HG12	4:R:115:PHE:CE2	2.56	0.40
5:E:71:LEU:C	5:E:71:LEU:HD22	2.47	0.40
15:g:1:00E:O	15:g:1:00E:CD2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	59
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	59
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	36
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	36
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
6	T	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
7	G	239/252 (95%)	234 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	238/252 (94%)	233 (98%)	5 (2%)	0	100	100
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	55
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	55
11	K	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	e	1/5 (20%)	1 (100%)	0	0	100	100
15	f	1/5 (20%)	1 (100%)	0	0	100	100
15	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6275/6630 (95%)	6096 (97%)	169 (3%)	10 (0%)	43	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
3	C	239	GLN
3	Q	239	GLN
3	C	205	ALA
10	J	2	ASP
3	Q	205	ALA
10	X	2	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	43	66
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	66
2	B	203/216 (94%)	194 (96%)	9 (4%)	25	54
2	P	203/216 (94%)	194 (96%)	9 (4%)	25	54
3	C	212/226 (94%)	205 (97%)	7 (3%)	33	60
3	Q	212/226 (94%)	205 (97%)	7 (3%)	33	60
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	39
4	R	194/215 (90%)	181 (93%)	13 (7%)	15	42
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	61
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	61
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	53
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	53
7	G	206/210 (98%)	200 (97%)	6 (3%)	37	63
7	U	206/210 (98%)	200 (97%)	6 (3%)	37	63
8	H	180/189 (95%)	174 (97%)	6 (3%)	33	60
8	V	180/189 (95%)	174 (97%)	6 (3%)	33	60
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	66
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	66
10	J	173/175 (99%)	169 (98%)	4 (2%)	44	66
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	66
11	K	168/168 (100%)	163 (97%)	5 (3%)	36	62
11	Y	168/168 (100%)	163 (97%)	5 (3%)	36	62
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	51
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	51
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	65
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	63	74
14	b	162/162 (100%)	160 (99%)	2 (1%)	63	74
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	0	1 (100%)	0	0
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	0	1 (100%)	0	0
All	All	5312/5540 (96%)	5129 (97%)	183 (3%)	32	60

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	102	ASN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	2	ARG
4	D	4	VAL
4	D	5	SER
4	D	20	LEU
4	D	40	LEU
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU

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Mol	Chain	Res	Type
4	D	176	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	188	LEU
6	F	14	ASP
6	F	68	ARG
6	F	78	ILE
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	9	ASN
8	H	13	VAL
8	H	34	LEU
8	H	38	SER
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	180	SER
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	144	LEU
10	J	174	MET
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	35	ILE
11	K	73	ARG
11	K	102	CYS
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	128	VAL
12	L	130	SER
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	119	VAL
1	O	17	LYS
1	O	29	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	2	ARG

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Mol	Chain	Res	Type
4	R	5	SER
4	R	20	LEU
4	R	40	LEU
4	R	60	VAL
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	188	LEU
6	T	14	ASP
6	T	68	ARG
6	T	78	ILE
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	9	ASN
8	V	13	VAL
8	V	34	LEU
8	V	38	SER
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	180	SER

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Mol	Chain	Res	Type
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	144	LEU
10	X	174	MET
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	102	CYS
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	106	TYR
12	Z	128	VAL
12	Z	130	SER
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	119	VAL
15	f	3	LEU
15	h	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	149	GLN
2	B	124	HIS
2	B	232	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	106	GLN
4	D	225	ASN

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Mol	Chain	Res	Type
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	178	HIS
6	F	240	GLN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	57	GLN
9	I	44	HIS
9	I	63	ASN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	208	ASN
12	L	70	ASN
12	L	79	HIS
12	L	108	HIS
12	L	158	ASN
12	L	197	GLN
13	M	26	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
14	N	141	ASN
1	O	30	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	232	GLN
3	Q	38	ASN
3	Q	147	GLN

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Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	233	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	147	GLN
5	S	184	ASN
6	T	86	ASN
6	T	123	ASN
6	T	240	GLN
7	U	30	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	57	GLN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
12	Z	197	GLN
13	a	26	ASN
13	a	102	GLN
14	b	28	ASN
14	b	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	00E	h	1	15	9,9,10	0.61	0	10,10,12	1.28	2 (20%)
15	00E	f	1	15	9,9,10	0.52	0	10,10,12	1.66	1 (10%)
15	HPE	f	2	15	11,12,13	1.52	1 (9%)	9,14,16	1.13	0
15	A1I67	h	5	15,11	13,19,20	2.07	3 (23%)	11,29,31	1.02	1 (9%)
15	A1JWF	h	4	15	5,10,11	2.01	1 (20%)	3,12,14	5.80	3 (100%)
15	HPE	e	2	15	11,12,13	1.72	1 (9%)	9,14,16	0.70	0
15	A1I67	f	5	15,11	13,19,20	1.88	5 (38%)	11,29,31	1.24	2 (18%)
15	A1I67	e	5	15,8	13,19,20	1.75	4 (30%)	11,29,31	1.12	1 (9%)
15	A1JWF	e	4	15	5,10,11	2.09	2 (40%)	3,12,14	5.85	3 (100%)
15	A1JWF	f	4	15	5,10,11	2.25	1 (20%)	3,12,14	5.99	3 (100%)
15	A1I67	g	5	15,8	13,19,20	2.31	4 (30%)	11,29,31	1.42	2 (18%)
15	HPE	h	2	15	11,12,13	1.56	1 (9%)	9,14,16	1.16	0
15	00E	e	1	15	9,9,10	0.58	0	10,10,12	1.64	1 (10%)
15	HPE	g	2	15	11,12,13	1.71	1 (9%)	9,14,16	0.65	0
15	A1JWF	g	4	15	5,10,11	1.20	1 (20%)	3,12,14	5.72	2 (66%)
15	00E	g	1	15	9,9,10	0.42	0	10,10,12	1.99	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	00E	h	1	15	-	0/2/11/12	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	HPE	f	2	15	-	3/6/7/9	0/1/1/1
15	A1I67	h	5	15,11	-	3/4/36/38	0/0/1/1
15	A1JWF	h	4	15	-	2/4/13/15	0/1/1/1
15	HPE	e	2	15	-	0/6/7/9	0/1/1/1
15	A1I67	f	5	15,11	-	3/4/36/38	0/0/1/1
15	A1I67	e	5	15,8	-	2/4/36/38	0/0/1/1
15	A1JWF	e	4	15	-	2/4/13/15	0/1/1/1
15	A1JWF	f	4	15	-	2/4/13/15	0/1/1/1
15	A1I67	g	5	15,8	-	2/4/36/38	0/0/1/1
15	HPE	h	2	15	-	4/6/7/9	0/1/1/1
15	00E	e	1	15	-	1/2/11/12	0/1/1/1
15	HPE	g	2	15	-	4/6/7/9	0/1/1/1
15	A1JWF	g	4	15	-	2/4/13/15	0/1/1/1
15	00E	g	1	15	-	1/2/11/12	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	5	A1I67	OG1-CB	-5.43	1.36	1.43
15	g	5	A1I67	OG1-CB	-5.16	1.36	1.43
15	e	2	HPE	CG-CD	-5.07	1.37	1.51
15	g	2	HPE	CG-CD	-4.94	1.37	1.51
15	h	2	HPE	CG-CD	-4.78	1.38	1.51
15	e	5	A1I67	OG1-CB	-4.51	1.37	1.43
15	f	2	HPE	CG-CD	-4.51	1.38	1.51
15	f	4	A1JWF	CB-CG	-4.19	1.49	1.51
15	g	5	A1I67	CB-CA	-4.05	1.47	1.53
15	f	5	A1I67	OG1-CB	-3.70	1.38	1.43
15	h	4	A1JWF	CB-CG	-3.70	1.49	1.51
15	e	4	A1JWF	CB-CG	-3.68	1.49	1.51
15	g	5	A1I67	OG1-C47	-3.58	1.36	1.43
15	h	5	A1I67	OG1-C47	-3.52	1.36	1.43
15	h	5	A1I67	O60-C51	-3.29	1.39	1.44
15	f	5	A1I67	O60-C51	-3.12	1.40	1.44
15	f	5	A1I67	OG1-C47	-2.95	1.37	1.43
15	g	5	A1I67	O60-C51	-2.75	1.40	1.44
15	e	5	A1I67	OG1-C47	-2.60	1.38	1.43
15	f	5	A1I67	C47-C42	-2.24	1.50	1.54
15	f	5	A1I67	CB-CA	-2.14	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	4	A1JWF	CE2-CD2	-2.11	1.32	1.42
15	g	4	A1JWF	CE2-CD2	-2.06	1.32	1.42
15	e	5	A1I67	CB-CA	-2.05	1.50	1.53
15	e	5	A1I67	O60-C51	-2.01	1.41	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	4	A1JWF	CB-CG-CD2	-8.62	123.35	133.97
15	f	4	A1JWF	CB-CG-CD2	-8.58	123.40	133.97
15	g	4	A1JWF	CB-CG-CD2	-8.46	123.55	133.97
15	h	4	A1JWF	CB-CG-CD2	-8.20	123.87	133.97
15	h	4	A1JWF	CE2-CD2-CG	5.08	118.96	107.16
15	g	4	A1JWF	CE2-CD2-CG	5.02	118.83	107.16
15	e	4	A1JWF	CE2-CD2-CG	4.89	118.54	107.16
15	f	4	A1JWF	CE2-CD2-CG	4.81	118.33	107.16
15	g	1	00E	CA-NB-CD1	-4.31	106.00	110.49
15	f	1	00E	CA-NB-CD1	-4.07	106.24	110.49
15	e	1	00E	CA-NB-CD1	3.80	114.46	110.49
15	g	1	00E	CA-NB-CD2	3.35	113.98	110.49
15	f	4	A1JWF	CA-CB-CG	-3.30	105.87	113.78
15	g	5	A1I67	CB-CA-N2	-3.12	104.74	111.75
15	h	4	A1JWF	CA-CB-CG	-2.81	107.04	113.78
15	f	5	A1I67	O48-C47-C51	2.73	112.65	106.08
15	h	5	A1I67	O48-C47-C51	2.72	112.62	106.08
15	e	5	A1I67	O48-C47-C51	2.66	112.47	106.08
15	h	1	00E	CA-NB-CD2	-2.36	108.03	110.49
15	h	1	00E	C-CA-NB	-2.33	108.34	112.80
15	g	5	A1I67	O48-C47-C51	2.22	111.42	106.08
15	f	5	A1I67	CB-CA-N2	-2.12	106.98	111.75
15	e	4	A1JWF	CA-CB-CG	-2.07	108.82	113.78

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	1	00E	C-CA-NB-CD1
15	g	1	00E	C-CA-NB-CD2
15	f	2	HPE	C-CA-CB-CG
15	g	2	HPE	C-CA-CB-CG
15	h	2	HPE	C-CA-CB-CG
15	e	4	A1JWF	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
15	f	4	A1JWF	C-CA-CB-CG
15	g	4	A1JWF	C-CA-CB-CG
15	h	4	A1JWF	C-CA-CB-CG
15	e	5	A1I67	N-C42-C43-C44
15	f	5	A1I67	N-C42-C43-C44
15	g	5	A1I67	N-C42-C43-C44
15	h	5	A1I67	N-C42-C43-C44
15	h	4	A1JWF	N-CA-CB-CG
15	h	5	A1I67	C42-C43-C44-C45
15	e	4	A1JWF	N-CA-CB-CG
15	f	4	A1JWF	N-CA-CB-CG
15	g	4	A1JWF	N-CA-CB-CG
15	f	5	A1I67	C47-C42-C43-C44
15	h	5	A1I67	C47-C42-C43-C44
15	g	2	HPE	N-CA-CB-CG
15	f	5	A1I67	C42-C43-C44-C45
15	f	2	HPE	CE2-CD-CG-CB
15	f	2	HPE	CE1-CD-CG-CB
15	e	5	A1I67	C47-C42-C43-C44
15	g	5	A1I67	C47-C42-C43-C44
15	h	2	HPE	CE2-CD-CG-CB
15	h	2	HPE	CE1-CD-CG-CB
15	g	2	HPE	CE1-CD-CG-CB
15	g	2	HPE	CE2-CD-CG-CB
15	h	2	HPE	N-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	h	1	00E	8	0
15	f	1	00E	3	0
15	f	2	HPE	1	0
15	h	5	A1I67	8	0
15	h	4	A1JWF	1	0
15	f	5	A1I67	3	0
15	f	4	A1JWF	1	0
15	g	5	A1I67	4	0
15	h	2	HPE	2	0
15	e	1	00E	1	0
15	g	1	00E	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	h	101	-	12,12,12	0.71	0	15,16,16	0.34	0
18	MES	f	101	-	12,12,12	0.73	0	15,16,16	0.38	0
18	MES	V	302	-	12,12,12	0.68	0	15,16,16	0.63	0
18	MES	H	301	-	12,12,12	0.72	0	15,16,16	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	h	101	-	-	0/6/14/14	0/1/1/1
18	MES	f	101	-	-	3/6/14/14	0/1/1/1
18	MES	V	302	-	-	6/6/14/14	0/1/1/1
18	MES	H	301	-	-	5/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	H	301	MES	C8-C7-N4-C3
18	H	301	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
18	H	301	MES	C7-C8-S-O1S
18	H	301	MES	C7-C8-S-O2S
18	H	301	MES	C7-C8-S-O3S
18	f	101	MES	C7-C8-S-O3S
18	V	302	MES	C7-C8-S-O3S
18	V	302	MES	C7-C8-S-O1S
18	V	302	MES	C7-C8-S-O2S
18	f	101	MES	C7-C8-S-O1S
18	f	101	MES	C7-C8-S-O2S
18	V	302	MES	N4-C7-C8-S
18	V	302	MES	C8-C7-N4-C3
18	V	302	MES	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	h	101	MES	1	0
18	V	302	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.30	1 (0%) 88 78	61, 75, 111, 166	0
1	O	250/250 (100%)	-0.26	1 (0%) 88 78	65, 85, 122, 152	0
2	B	244/258 (94%)	-0.11	0 100 100	61, 82, 130, 161	0
2	P	244/258 (94%)	0.00	2 (0%) 82 66	64, 87, 139, 166	0
3	C	240/254 (94%)	-0.19	0 100 100	62, 85, 136, 148	0
3	Q	240/254 (94%)	-0.06	3 (1%) 75 55	69, 100, 156, 171	0
4	D	235/260 (90%)	-0.19	1 (0%) 88 78	63, 85, 110, 145	0
4	R	235/260 (90%)	-0.15	0 100 100	65, 94, 125, 156	0
5	E	231/234 (98%)	-0.19	0 100 100	64, 90, 117, 142	0
5	S	231/234 (98%)	-0.09	0 100 100	67, 98, 134, 155	0
6	F	243/288 (84%)	-0.23	1 (0%) 88 78	59, 81, 117, 150	0
6	T	243/288 (84%)	-0.20	1 (0%) 88 78	65, 88, 124, 147	0
7	G	241/252 (95%)	-0.17	0 100 100	53, 77, 107, 151	0
7	U	240/252 (95%)	-0.24	0 100 100	61, 80, 107, 137	0
8	H	221/231 (95%)	-0.26	0 100 100	57, 73, 98, 138	0
8	V	221/231 (95%)	-0.25	0 100 100	60, 76, 96, 139	0
9	I	204/205 (99%)	-0.33	0 100 100	57, 71, 95, 114	0
9	W	204/205 (99%)	-0.38	0 100 100	56, 72, 96, 115	0
10	J	195/198 (98%)	-0.38	1 (0%) 87 75	55, 72, 97, 121	0
10	X	195/198 (98%)	-0.40	1 (0%) 87 75	58, 76, 97, 127	0
11	K	211/211 (100%)	-0.36	0 100 100	58, 73, 94, 118	0
11	Y	211/211 (100%)	-0.31	0 100 100	60, 77, 98, 124	0
12	L	222/222 (100%)	-0.30	1 (0%) 87 75	56, 74, 97, 114	0
12	Z	222/222 (100%)	-0.24	0 100 100	58, 77, 100, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.32	1 (0%) 88 78	57, 75, 95, 108	0
13	a	233/246 (94%)	-0.37	1 (0%) 88 78	54, 72, 92, 102	0
14	N	196/196 (100%)	-0.34	0 100 100	48, 69, 95, 115	0
14	b	196/196 (100%)	-0.31	0 100 100	51, 71, 97, 121	0
15	e	1/5 (20%)	0.83	0 100 100	72, 72, 72, 72	0
15	f	1/5 (20%)	0.30	0 100 100	80, 80, 80, 80	0
15	g	1/5 (20%)	1.08	0 100 100	75, 75, 75, 75	0
15	h	1/5 (20%)	0.41	0 100 100	83, 83, 83, 83	0
All	All	6335/6630 (95%)	-0.24	15 (0%) 91 84	48, 79, 120, 171	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	3.2
10	J	1	MET	3.0
1	A	1	MET	2.7
4	D	117	GLU	2.7
13	a	1	THR	2.6
2	P	51	VAL	2.5
3	Q	189	CYS	2.5
10	X	1	MET	2.5
13	M	1	THR	2.4
12	L	136	CYS	2.3
6	F	215	CYS	2.3
3	Q	205	ALA	2.2
2	P	212	PHE	2.1
3	Q	50	LEU	2.1
6	T	72	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	HPE	h	2	12/13	0.68	0.24	90,101,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	A1JWF	e	4	10/11	0.73	0.34	42,45,65,67	0
15	A1JWF	g	4	10/11	0.73	0.36	41,45,66,67	0
15	HPE	f	2	12/13	0.74	0.24	88,103,105,107	0
15	A1JWF	f	4	10/11	0.77	0.34	46,51,63,71	0
15	00E	f	1	9/10	0.78	0.19	96,120,129,129	0
15	A1JWF	h	4	10/11	0.79	0.34	49,53,66,71	0
15	HPE	g	2	12/13	0.80	0.14	76,78,79,84	0
15	00E	h	1	9/10	0.80	0.18	99,116,121,122	0
15	00E	g	1	9/10	0.83	0.20	86,111,114,114	0
15	HPE	e	2	12/13	0.85	0.15	78,82,83,85	0
15	00E	e	1	9/10	0.89	0.18	87,100,102,102	0
15	A1I67	g	5	19/20	0.90	0.17	70,73,79,83	0
15	A1I67	h	5	19/20	0.92	0.12	67,72,73,74	0
15	A1I67	f	5	19/20	0.94	0.10	63,68,71,74	0
15	A1I67	e	5	19/20	0.95	0.12	69,72,79,85	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	I	301	1/1	0.57	0.46	126,126,126,126	0
18	MES	V	302	12/12	0.77	0.25	129,144,147,149	0
18	MES	H	301	12/12	0.83	0.21	113,122,124,124	0
16	MG	Y	301	1/1	0.84	0.11	103,103,103,103	0
18	MES	f	101	12/12	0.91	0.17	100,102,108,112	0
18	MES	h	101	12/12	0.91	0.15	94,97,106,108	0
16	MG	Z	301	1/1	0.92	0.22	83,83,83,83	0
16	MG	V	301	1/1	0.95	0.10	107,107,107,107	0
17	CL	b	201	1/1	0.95	0.13	108,108,108,108	0
16	MG	K	301	1/1	0.96	0.10	89,89,89,89	0
17	CL	N	202	1/1	0.98	0.06	89,89,89,89	0
16	MG	N	201	1/1	0.98	0.13	60,60,60,60	0
16	MG	G	301	1/1	0.98	0.04	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CL	U	301	1/1	0.99	0.07	69,69,69,69	0
17	CL	G	302	1/1	0.99	0.06	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.