Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 01:01 PM EDT

PDB ID	:	1OS9
Title	:	Binary enzyme-product complexes of human MMP12
Authors	:	Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Mangani, S.; Terni, B.
Deposited on	:	2003-03-19
Resolution	:	1.85 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 (i) 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 (1)) were used in the production of this report:

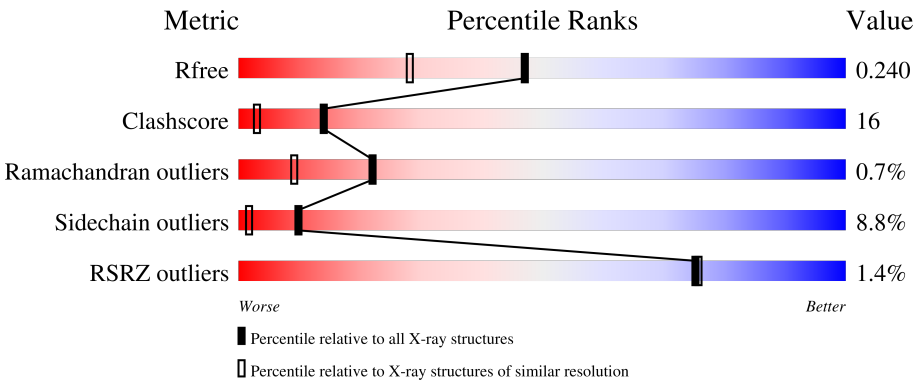
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	165	2% 72% 22% 5% •
1	B	165	2% 75% 21% • •
1	C	165	% 72% 22% 6% •
1	D	165	% 75% 21% • •
1	E	165	2% 76% 16% 7% •

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Mol	Chain	Length	Quality of chain
1	F	165	% 79% 16% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8677 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1295	823	225	242	5	0	7	0
1	B	165	1295	823	225	242	5	0	6	0
1	C	165	1295	823	225	242	5	0	7	0
1	D	165	1295	823	225	242	5	0	7	0
1	E	165	1295	823	225	242	5	0	7	0
1	F	165	1295	823	225	242	5	0	7	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	cloning artifact	UNP P39900
A	105	MET	-	cloning artifact	UNP P39900
A	171	ASP	PHE	engineered mutation	UNP P39900
B	104	MET	-	cloning artifact	UNP P39900
B	105	MET	-	cloning artifact	UNP P39900
B	171	ASP	PHE	engineered mutation	UNP P39900
C	104	MET	-	cloning artifact	UNP P39900
C	105	MET	-	cloning artifact	UNP P39900
C	171	ASP	PHE	engineered mutation	UNP P39900
D	104	MET	-	cloning artifact	UNP P39900
D	105	MET	-	cloning artifact	UNP P39900
D	171	ASP	PHE	engineered mutation	UNP P39900
E	104	MET	-	cloning artifact	UNP P39900
E	105	MET	-	cloning artifact	UNP P39900
E	171	ASP	PHE	engineered mutation	UNP P39900
F	104	MET	-	cloning artifact	UNP P39900
F	105	MET	-	cloning artifact	UNP P39900

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Chain	Residue	Modelled	Actual	Comment	Reference
F	171	ASP	PHE	engineered mutation	UNP P39900

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	B	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	E	3	Total Ca 3 3	0	0
3	F	3	Total Ca 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	158	Total O 158 158	0	0

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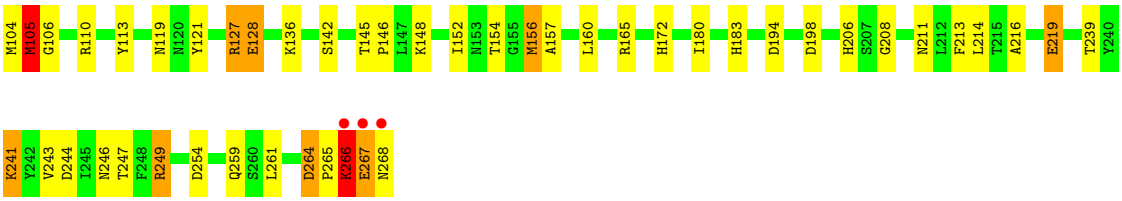
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	150	150	150	0	0
			Total	O		
4	D	146	146	146	0	0
			Total	O		
4	E	122	122	122	0	0
			Total	O		
4	F	124	124	124	0	0

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.

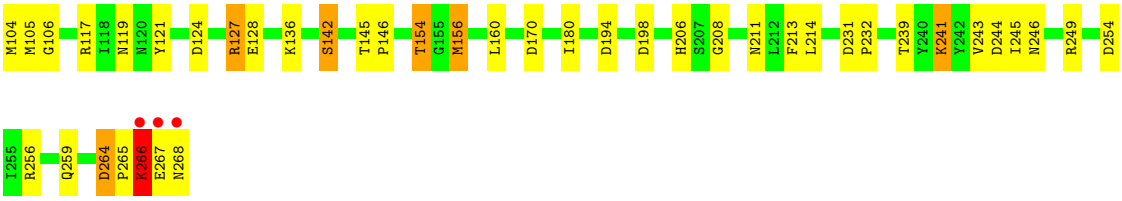
• Molecule 1: Macrophage metalloelastase

Chain A:



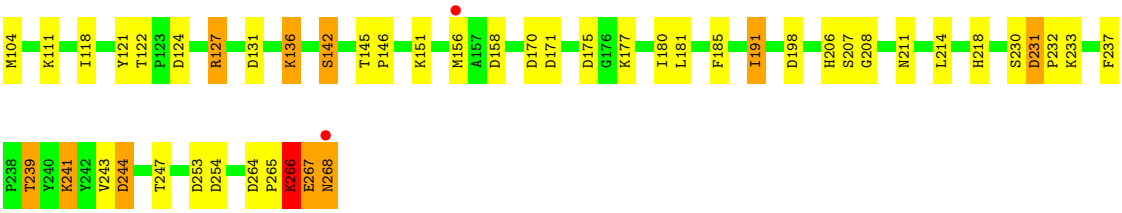
• Molecule 1: Macrophage metalloelastase

Chain B:



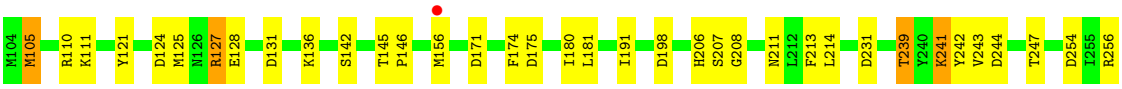
• Molecule 1: Macrophage metalloelastase

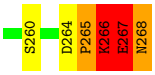
Chain C:



• Molecule 1: Macrophage metalloelastase

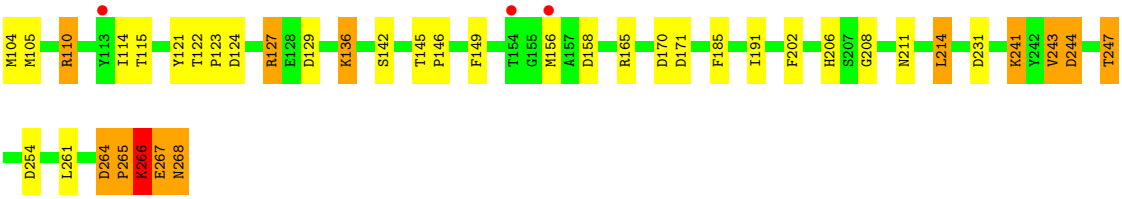
Chain D:





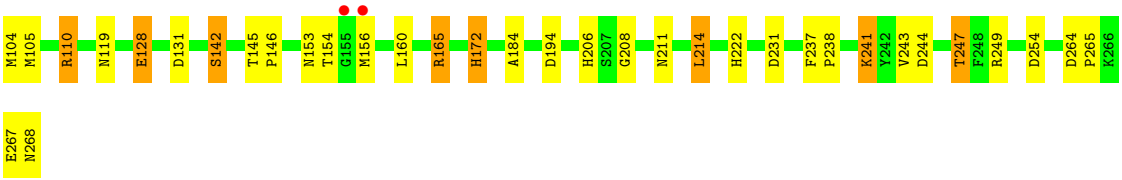
• Molecule 1: Macrophage metalloelastase

Chain E:



• Molecule 1: Macrophage metalloelastase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	125.44Å 125.44Å 72.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 1.85 19.83 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-1.85) 99.9 (19.83-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.80	Depositor
R, R_{free}	0.195 , 0.244 0.199 , 0.240	Depositor DCC
R_{free} test set	5422 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.480 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8677	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	1.08	2/1333 (0.2%)	1.10	7/1805 (0.4%)
1	B	1.10	0/1333	1.10	5/1805 (0.3%)
1	C	1.02	0/1333	1.16	14/1805 (0.8%)
1	D	1.12	4/1333 (0.3%)	1.42	21/1805 (1.2%)
1	E	0.95	0/1333	1.06	9/1805 (0.5%)
1	F	0.94	0/1333	1.01	4/1805 (0.2%)
All	All	1.04	6/7998 (0.1%)	1.15	60/10830 (0.6%)

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
1	A	0	1
1	B	0	1
1	D	0	3
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	LYS	C-N	7.56	1.51	1.34
1	D	264	ASP	C-N	7.28	1.48	1.34
1	D	174	PHE	CE1-CZ	5.71	1.48	1.37
1	D	267	GLU	C-O	5.50	1.33	1.23
1	A	219	GLU	CD-OE1	-5.41	1.19	1.25
1	A	216	ALA	CA-CB	5.03	1.63	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	266	LYS	C-N-CA	20.32	172.51	121.70
1	D	267	GLU	C-N-CA	13.51	155.47	121.70
1	D	265	PRO	C-N-CA	11.56	150.59	121.70
1	D	268	ASN	N-CA-CB	11.52	131.33	110.60
1	D	231	ASP	CB-CG-OD2	9.57	126.91	118.30
1	D	265	PRO	CA-C-N	9.08	137.18	117.20
1	D	264	ASP	CB-CG-OD2	8.79	126.21	118.30
1	C	175	ASP	CB-CG-OD2	8.67	126.10	118.30
1	C	231	ASP	CB-CG-OD2	8.22	125.70	118.30
1	B	194	ASP	CB-CG-OD2	8.16	125.65	118.30
1	D	267	GLU	O-C-N	-7.44	110.79	122.70
1	D	254	ASP	CB-CG-OD2	7.34	124.90	118.30
1	D	171	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	194	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	264	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	171	ASP	CB-CG-OD2	7.08	124.67	118.30
1	C	254	ASP	CB-CG-OD2	6.99	124.59	118.30
1	D	267	GLU	CA-C-N	6.98	132.56	117.20
1	E	129	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	165	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	267	GLU	OE1-CD-OE2	-6.45	115.57	123.30
1	E	254	ASP	CB-CG-OD2	6.44	124.09	118.30
1	D	124	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	239	THR	OG1-CB-CG2	-6.41	95.26	110.00
1	E	264	ASP	CB-CG-OD2	6.33	123.99	118.30
1	C	131	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	175	ASP	CB-CG-OD2	6.28	123.95	118.30
1	F	231	ASP	CB-CG-OD2	6.28	123.95	118.30
1	E	171	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	253	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	254	ASP	CB-CG-OD2	6.22	123.90	118.30
1	D	131	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	198	ASP	CB-CG-OD2	6.11	123.80	118.30
1	F	254	ASP	CB-CG-OD2	6.06	123.75	118.30
1	F	131	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	198	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	198	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	265	PRO	O-C-N	-5.77	113.46	122.70
1	B	254	ASP	CB-CG-OD2	5.73	123.46	118.30
1	E	170	ASP	CB-CG-OD2	5.68	123.41	118.30
1	E	265	PRO	C-N-CA	5.57	135.63	121.70
1	F	194	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	165	ARG	NE-CZ-NH1	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	170	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	128	GLU	CB-CA-C	-5.38	99.64	110.40
1	E	244	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	156	MET	CB-CA-C	5.33	121.05	110.40
1	D	156	MET	CB-CA-C	5.31	121.03	110.40
1	A	105	MET	CB-CA-C	5.31	121.01	110.40
1	D	266	LYS	CB-CA-C	5.29	120.97	110.40
1	C	124	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	198	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	110[A]	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	244	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	171	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	B	170	ASP	CB-CG-OD1	5.15	122.93	118.30
1	E	243	VAL	CB-CA-C	-5.12	101.66	111.40
1	C	158	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	231	ASP	CB-CG-OD2	5.08	122.87	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LYS	Peptide
1	B	266	LYS	Peptide
1	D	266	LYS	Peptide
1	D	267	GLU	Peptide,Mainchain

5.2 Too-close contacts (i)

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	1295	0	1210	52	1
1	B	1295	0	1210	46	0
1	C	1295	0	1210	46	0
1	D	1295	0	1208	29	0
1	E	1295	0	1210	44	0
1	F	1295	0	1210	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	177	0	0	14	0
4	B	158	0	0	9	0
4	C	150	0	0	8	0
4	D	146	0	0	7	0
4	E	122	0	0	7	0
4	F	124	0	0	4	1
All	All	8677	0	7258	238	1

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 16.

All (238) 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)
1:E:266:LYS:HB3	4:E:1029:HOH:O	1.39	1.23
1:A:160:LEU:HB2	4:A:1069:HOH:O	1.43	1.17
1:A:265:PRO:HA	1:A:266:LYS:HB2	1.26	1.12
1:C:265:PRO:HA	1:C:266:LYS:HB2	1.16	1.11
1:A:241[A]:LYS:HE3	1:A:243:VAL:HG13	1.31	1.09
1:B:265:PRO:CA	1:B:266:LYS:HB2	1.82	1.08
1:A:265:PRO:CA	1:A:266:LYS:HB2	1.84	1.08
1:B:265:PRO:HA	1:B:266:LYS:HB2	1.29	1.07
1:C:265:PRO:CA	1:C:266:LYS:HB2	1.88	1.03
1:B:136:LYS:HD3	1:B:245:ILE:HD11	1.41	1.02
1:D:206:HIS:HD2	1:D:208:GLY:H	1.09	0.96
1:E:267:GLU:HA	1:E:268:ASN:CB	1.96	0.96
1:D:206:HIS:CD2	1:D:208:GLY:H	1.85	0.93
1:B:267:GLU:HB2	1:B:268:ASN:HB2	1.50	0.92
1:C:185:PHE:CE1	1:C:191:ILE:HD11	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:O	1:B:156:MET:HE3	1.71	0.91
1:A:148:LYS:HE2	4:A:1068:HOH:O	1.72	0.90
1:E:267:GLU:O	1:E:267:GLU:HG2	1.71	0.90
1:C:206:HIS:CD2	1:C:208:GLY:H	1.90	0.89
1:E:267:GLU:CA	1:E:268:ASN:HB2	2.03	0.88
1:A:156:MET:HE3	1:A:156:MET:O	1.76	0.85
1:B:206:HIS:HD2	1:B:208:GLY:H	1.22	0.85
1:C:244:ASP:HB3	1:C:247:THR:HG22	1.56	0.84
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.43	0.84
1:E:206:HIS:HD2	1:E:208:GLY:H	1.22	0.83
1:F:267:GLU:HB2	1:F:268:ASN:HB2	1.61	0.83
1:B:265:PRO:HA	1:B:266:LYS:CB	2.05	0.81
1:C:185:PHE:CZ	1:C:191:ILE:HD11	2.15	0.81
1:E:267:GLU:O	1:E:267:GLU:CG	2.29	0.80
1:B:265:PRO:CB	1:B:266:LYS:HB2	2.11	0.79
1:A:219:GLU:OE2	1:E:104:MET:N	2.15	0.79
1:A:206:HIS:HD2	1:A:208:GLY:H	1.32	0.77
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.50	0.77
1:D:211[A]:ASN:HD22	1:D:214:LEU:H	1.32	0.77
1:C:211[A]:ASN:HD22	1:C:214:LEU:H	1.33	0.75
1:B:136:LYS:CD	1:B:245:ILE:HD11	2.16	0.73
1:B:241[A]:LYS:HE2	1:B:243:VAL:HG13	1.71	0.73
1:B:266:LYS:HE2	1:B:266:LYS:HA	1.70	0.73
1:A:265:PRO:CB	1:A:266:LYS:HB2	2.19	0.72
1:A:265:PRO:HA	1:A:266:LYS:CB	2.10	0.72
1:C:206:HIS:HD2	1:C:208:GLY:H	1.35	0.72
1:E:267:GLU:HA	1:E:268:ASN:HB2	1.61	0.72
1:A:267:GLU:HG3	1:A:267:GLU:O	1.91	0.71
1:F:267:GLU:CB	1:F:268:ASN:HB2	2.20	0.71
1:E:110[A]:ARG:HG2	4:E:1000:HOH:O	1.91	0.71
1:C:136:LYS:HE3	4:C:1007:HOH:O	1.89	0.71
1:C:266:LYS:HD3	4:C:955:HOH:O	1.90	0.70
1:E:244:ASP:HB3	1:E:247:THR:HG22	1.73	0.70
1:F:267:GLU:HB2	1:F:268:ASN:CB	2.20	0.70
1:F:119:ASN:HB2	1:F:160:LEU:HD11	1.74	0.70
1:B:266:LYS:HA	1:B:266:LYS:CE	2.23	0.69
1:C:233:LYS:HB2	1:C:233:LYS:NZ	2.08	0.69
1:F:206:HIS:HD2	1:F:208:GLY:H	1.38	0.69
1:B:156:MET:O	1:B:156:MET:CE	2.41	0.68
1:A:136:LYS:HD2	4:A:1017:HOH:O	1.93	0.68
1:F:244:ASP:HB3	1:F:247:THR:CG2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241[A]:LYS:HE3	1:A:243:VAL:CG1	2.18	0.66
1:C:265:PRO:CA	1:C:266:LYS:CB	2.72	0.66
1:B:206:HIS:CD2	1:B:208:GLY:H	2.09	0.65
1:C:146[A]:PRO:HB3	1:C:266:LYS:HD2	1.78	0.65
1:A:104:MET:N	4:A:1079:HOH:O	2.29	0.64
1:E:206:HIS:CD2	1:E:208:GLY:H	2.11	0.64
1:E:265:PRO:HA	1:E:266:LYS:HB2	1.81	0.63
1:B:267:GLU:CB	1:B:268:ASN:HB2	2.28	0.63
1:D:127:ARG:HG3	1:D:127:ARG:NH1	2.10	0.63
1:F:244:ASP:HB3	1:F:247:THR:HG22	1.81	0.63
1:C:145:THR:HB	1:C:146[A]:PRO:HD2	1.80	0.62
1:E:267:GLU:HA	1:E:268:ASN:CG	2.19	0.62
1:B:239:THR:HG22	1:F:105:MET:HB3	1.81	0.62
1:D:244:ASP:HB3	1:D:247:THR:HG22	1.80	0.62
1:B:256:ARG:HG2	1:B:256:ARG:NH2	2.15	0.62
1:E:244:ASP:HB3	1:E:247:THR:CG2	2.30	0.62
1:B:136:LYS:HG2	1:B:213:PHE:CE2	2.36	0.61
1:F:110[A]:ARG:HG2	4:F:969:HOH:O	2.00	0.61
1:C:265:PRO:HA	1:C:266:LYS:CB	2.09	0.61
1:A:136:LYS:HD2	4:A:1018:HOH:O	2.00	0.61
1:C:180:ILE:HD12	4:C:995:HOH:O	2.01	0.60
1:D:241[A]:LYS:HE2	1:D:243:VAL:HG13	1.84	0.60
1:D:211[A]:ASN:ND2	1:D:214:LEU:H	1.99	0.59
1:C:211[A]:ASN:ND2	1:C:214:LEU:H	1.99	0.59
1:E:247:THR:HG21	4:E:1045:HOH:O	2.02	0.59
1:E:267:GLU:HA	1:E:268:ASN:ND2	2.17	0.59
1:E:267:GLU:CA	1:E:268:ASN:CB	2.63	0.59
1:A:206:HIS:CD2	1:A:208:GLY:H	2.19	0.58
1:C:244:ASP:HB3	1:C:247:THR:CG2	2.28	0.58
1:D:211[A]:ASN:HD21	1:D:213:PHE:HB3	1.68	0.58
1:D:180:ILE:CD1	4:D:980:HOH:O	2.51	0.58
1:A:265:PRO:CA	1:A:266:LYS:CB	2.66	0.57
1:C:267:GLU:CB	1:C:268:ASN:HA	2.33	0.57
1:C:127:ARG:HG3	1:C:127:ARG:NH1	2.19	0.57
1:A:259:GLN:CD	1:A:264:ASP:HB3	2.25	0.56
1:C:118:ILE:HD12	1:C:151:LYS:HE2	1.87	0.56
1:C:266:LYS:HE2	4:C:1026:HOH:O	2.05	0.56
1:E:211[A]:ASN:HD22	1:E:214:LEU:H	1.54	0.56
1:B:241[A]:LYS:HE2	1:B:243:VAL:CG1	2.36	0.56
1:E:127:ARG:HH11	1:E:127:ARG:CG	2.19	0.55
1:A:211[A]:ASN:HD22	1:A:214:LEU:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LYS:C	4:C:990:HOH:O	2.44	0.55
1:E:136:LYS:HG3	4:E:1043:HOH:O	2.07	0.55
1:F:145:THR:HB	1:F:146[A]:PRO:CD	2.37	0.55
1:A:214:LEU:HD11	1:A:243:VAL:O	2.06	0.54
1:F:243:VAL:HG12	1:F:247:THR:HG23	1.89	0.54
1:C:180:ILE:CD1	4:C:995:HOH:O	2.54	0.54
1:E:267:GLU:CB	1:E:268:ASN:HB2	2.38	0.54
1:A:145:THR:HB	1:A:146[A]:PRO:HD2	1.88	0.54
1:E:127:ARG:NH1	1:E:127:ARG:HG3	2.21	0.54
1:F:211[A]:ASN:HD22	1:F:214:LEU:H	1.56	0.54
1:F:206:HIS:CD2	1:F:208:GLY:H	2.23	0.54
4:A:963:HOH:O	1:C:239:THR:HG21	2.08	0.53
1:B:214:LEU:HD11	1:B:243:VAL:O	2.08	0.53
1:D:145:THR:HB	1:D:146[A]:PRO:HD2	1.90	0.53
1:C:267:GLU:HB2	1:C:268:ASN:HA	1.91	0.53
1:A:239:THR:HG22	1:E:105:MET:HB3	1.90	0.53
1:F:244:ASP:HB3	1:F:247:THR:HG21	1.91	0.53
1:B:211[A]:ASN:HD22	1:B:214:LEU:H	1.57	0.53
1:D:244:ASP:HB3	1:D:247:THR:CG2	2.38	0.53
1:C:214:LEU:HD11	1:C:243:VAL:H	1.74	0.52
1:C:233:LYS:NZ	1:C:233:LYS:CB	2.72	0.52
1:D:180:ILE:HD12	4:D:980:HOH:O	2.10	0.52
1:A:136:LYS:CD	4:A:1018:HOH:O	2.58	0.52
1:B:117:ARG:NH1	1:B:154:THR:HA	2.24	0.52
1:A:136:LYS:CD	4:A:1017:HOH:O	2.57	0.52
1:E:121:TYR:CE1	1:E:127:ARG:HG2	2.45	0.51
1:E:243:VAL:HG12	1:E:247:THR:HG23	1.91	0.51
1:F:172:HIS:N	1:F:172:HIS:CD2	2.78	0.51
1:A:156:MET:HE1	4:A:991:HOH:O	2.10	0.51
1:A:105:MET:HG3	1:A:261:LEU:HD21	1.93	0.51
1:C:185:PHE:CZ	1:C:191:ILE:CD1	2.89	0.50
1:B:259:GLN:CD	1:B:264:ASP:HB3	2.31	0.50
1:E:145:THR:HB	1:E:146[A]:PRO:CD	2.41	0.50
1:A:180:ILE:HD12	4:A:971:HOH:O	2.11	0.50
1:C:266:LYS:HB3	4:C:943:HOH:O	2.11	0.50
1:D:121:TYR:CE1	1:D:127:ARG:HG2	2.46	0.50
1:E:105:MET:SD	4:E:1010:HOH:O	2.60	0.50
1:A:106:GLY:HA2	1:C:181:LEU:HD11	1.93	0.50
1:C:233:LYS:CB	1:C:233:LYS:HZ3	2.25	0.50
1:E:185:PHE:CE1	1:E:191:ILE:HD11	2.47	0.50
1:A:146[A]:PRO:HB3	1:A:266:LYS:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:HIS:CD2	1:D:207:SER:N	2.81	0.49
1:B:119:ASN:HB2	1:B:160:LEU:HD11	1.93	0.49
1:B:256:ARG:HG2	1:B:256:ARG:HH21	1.78	0.48
1:E:127:ARG:CG	1:E:127:ARG:NH1	2.77	0.48
1:E:264:ASP:HB2	1:E:265:PRO:CD	2.43	0.47
1:F:128:GLU:HG3	4:F:975:HOH:O	2.13	0.47
1:A:249:ARG:HH21	1:A:249:ARG:HG3	1.80	0.47
1:B:259:GLN:OE1	1:B:264:ASP:CB	2.62	0.47
1:A:244:ASP:OD2	1:A:246:ASN:HB2	2.14	0.47
1:A:266:LYS:HA	1:A:266:LYS:HE2	1.97	0.47
1:A:119:ASN:HB2	1:A:160:LEU:HD11	1.97	0.47
1:B:156:MET:CE	4:B:983:HOH:O	2.62	0.46
1:B:136:LYS:CD	4:B:1032:HOH:O	2.63	0.46
1:E:268:ASN:ND2	4:E:1024:HOH:O	2.41	0.46
1:F:142[A]:SER:HB3	4:F:952:HOH:O	2.14	0.46
1:C:233:LYS:HB2	1:C:233:LYS:HZ2	1.81	0.46
1:C:233:LYS:HB2	1:C:233:LYS:HZ3	1.79	0.46
1:F:145:THR:HB	1:F:146[A]:PRO:HD2	1.97	0.46
1:A:127:ARG:NH1	1:A:127:ARG:HG3	2.31	0.46
1:B:106:GLY:HA2	1:D:181:LEU:HD11	1.98	0.46
1:C:142[A]:SER:HB3	4:C:970:HOH:O	2.15	0.46
1:F:104:MET:N	4:F:946:HOH:O	2.49	0.45
1:A:249:ARG:HH21	1:A:249:ARG:CG	2.29	0.45
1:B:105:MET:HB2	1:D:239:THR:HG22	1.98	0.45
1:C:241[A]:LYS:HE2	1:C:241[A]:LYS:HB3	1.76	0.45
1:D:180:ILE:HD13	4:D:975:HOH:O	2.15	0.45
1:E:241[A]:LYS:HE3	1:E:243:VAL:HG22	1.99	0.45
1:B:156:MET:HE1	4:B:983:HOH:O	2.17	0.45
1:F:244:ASP:O	1:F:247:THR:HG22	2.15	0.45
1:B:259:GLN:OE1	1:B:264:ASP:HB2	2.17	0.44
1:B:136:LYS:CG	4:B:1032:HOH:O	2.65	0.44
1:E:115:THR:O	1:E:158:ASP:HB2	2.17	0.44
1:E:124:ASP:HB3	1:E:202:PHE:CE1	2.52	0.44
1:F:241[A]:LYS:HE3	1:F:243:VAL:HG22	1.99	0.44
1:D:105:MET:HE2	1:D:105:MET:HB2	1.55	0.44
1:D:125:MET:HG2	4:D:1010:HOH:O	2.18	0.44
1:D:191:ILE:HD12	4:D:956:HOH:O	2.18	0.43
1:B:104:MET:N	4:B:1054:HOH:O	2.51	0.43
1:B:244:ASP:OD2	1:B:246:ASN:N	2.44	0.43
1:E:266:LYS:CB	4:E:1029:HOH:O	2.21	0.43
1:A:136:LYS:CE	4:A:1018:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:HIS:HB2	1:A:183[A]:HIS:CE1	2.54	0.43
1:B:231:ASP:HA	1:B:232:PRO:HD2	1.90	0.43
1:F:237:PHE:HA	1:F:238:PRO:HD3	1.81	0.43
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.83	0.43
1:B:121:TYR:CE1	1:B:127:ARG:HG2	2.54	0.43
1:D:136:LYS:HE2	4:D:967:HOH:O	2.19	0.43
1:B:142[A]:SER:HB3	4:B:943:HOH:O	2.19	0.43
1:E:267:GLU:HB2	1:E:268:ASN:HD22	1.83	0.43
1:B:145:THR:HB	1:B:146[A]:PRO:HD2	2.01	0.42
1:B:264:ASP:HB2	1:B:265:PRO:CD	2.49	0.42
1:E:105:MET:HG2	1:E:261:LEU:HD21	2.01	0.42
1:F:264:ASP:HB2	1:F:265:PRO:CD	2.49	0.42
1:A:121:TYR:CE1	1:A:127:ARG:HG2	2.54	0.42
1:A:156:MET:HE3	1:A:156:MET:C	2.39	0.42
1:A:156:MET:HA	4:A:1038:HOH:O	2.19	0.42
1:B:180:ILE:HD12	4:B:954:HOH:O	2.19	0.42
1:C:265:PRO:CB	1:C:266:LYS:HB2	2.47	0.42
1:F:184:ALA:HB3	1:F:222:HIS:HB2	2.01	0.42
1:B:206:HIS:HE1	4:B:951:HOH:O	2.03	0.42
1:E:122:THR:HA	1:E:123:PRO:HD2	1.80	0.42
1:E:265:PRO:HA	1:E:266:LYS:CB	2.49	0.42
1:A:136:LYS:HB2	4:A:1017:HOH:O	2.19	0.42
1:B:244:ASP:OD2	1:B:246:ASN:HB2	2.20	0.42
1:C:206:HIS:CD2	1:C:207:SER:N	2.87	0.42
1:D:191:ILE:CD1	4:D:956:HOH:O	2.67	0.42
1:A:211[A]:ASN:HD21	1:A:213:PHE:HB3	1.85	0.42
1:D:207:SER:HB3	1:D:242:TYR:CE2	2.55	0.42
1:D:191:ILE:O	1:D:191:ILE:HG13	2.20	0.41
1:E:114:ILE:O	1:E:149:PHE:HA	2.19	0.41
1:B:127:ARG:NH1	4:B:1047:HOH:O	2.54	0.41
1:C:231:ASP:HA	1:C:232:PRO:HD2	1.93	0.41
1:C:121:TYR:CE1	1:C:127:ARG:HG2	2.55	0.41
1:D:241[A]:LYS:CE	1:D:243:VAL:HG13	2.49	0.41
1:D:105:MET:HB3	1:D:105:MET:HE3	1.72	0.41
1:B:156:MET:HB3	1:B:156:MET:HE2	1.56	0.41
1:F:165:ARG:HH11	1:F:165:ARG:HD2	1.73	0.41
1:B:127:ARG:NH1	1:B:127:ARG:HG3	2.36	0.41
1:A:152:ILE:HD11	1:A:157:ALA:HB2	2.03	0.41
1:A:160:LEU:HD11	4:A:1072:HOH:O	2.21	0.41
1:D:244:ASP:O	1:D:247:THR:HG22	2.21	0.41
1:A:259:GLN:OE1	1:A:264:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PRO:CB	1:A:266:LYS:CB	2.93	0.40
1:D:206:HIS:CD2	1:D:208:GLY:N	2.70	0.40
1:A:104:MET:HB2	1:C:218:HIS:CD2	2.57	0.40
1:E:206:HIS:HD2	1:E:208:GLY:N	2.04	0.40
1:F:244:ASP:CB	1:F:247:THR:HG22	2.49	0.40
1:A:267:GLU:HA	1:A:268:ASN:HA	1.90	0.40
1:C:185:PHE:CE1	1:C:191:ILE:CD1	2.92	0.40
1:C:232:PRO:HA	1:C:237:PHE:CG	2.57	0.40
1:C:232:PRO:HA	1:C:237:PHE:CD1	2.56	0.40
1:C:136:LYS:HE2	1:C:136:LYS:HB3	1.13	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:OH	4:F:943:HOH:O[2_755]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	163/165 (99%)	157 (96%)	5 (3%)	1 (1%)	25 12
1	B	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	25 12
1	C	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	25 12
1	D	163/165 (99%)	157 (96%)	3 (2%)	3 (2%)	8 2
1	E	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	25 12
1	F	163/165 (99%)	160 (98%)	3 (2%)	0	100 100
All	All	978/990 (99%)	948 (97%)	23 (2%)	7 (1%)	22 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	266	LYS
1	D	266	LYS
1	D	267	GLU
1	E	266	LYS
1	A	266	LYS
1	B	266	LYS
1	D	265	PRO

5.3.2 Protein sidechains (i)

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	134/134 (100%)	121 (90%)	13 (10%)	8 1
1	B	134/134 (100%)	125 (93%)	9 (7%)	16 4
1	C	134/134 (100%)	121 (90%)	13 (10%)	8 1
1	D	134/134 (100%)	122 (91%)	12 (9%)	9 1
1	E	134/134 (100%)	122 (91%)	12 (9%)	9 1
1	F	134/134 (100%)	122 (91%)	12 (9%)	9 1
All	All	804/804 (100%)	733 (91%)	71 (9%)	10 2

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	MET
1	A	110[A]	ARG
1	A	127	ARG
1	A	128	GLU
1	A	142[A]	SER
1	A	154	THR
1	A	156	MET
1	A	241[A]	LYS
1	A	247	THR
1	A	249	ARG
1	A	264	ASP
1	A	266	LYS

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Mol	Chain	Res	Type
1	A	267	GLU
1	B	127	ARG
1	B	128	GLU
1	B	142[A]	SER
1	B	154	THR
1	B	156	MET
1	B	241[A]	LYS
1	B	249	ARG
1	B	264	ASP
1	B	266	LYS
1	C	104	MET
1	C	111	LYS
1	C	122	THR
1	C	127	ARG
1	C	136	LYS
1	C	142[A]	SER
1	C	177	LYS
1	C	191	ILE
1	C	230	SER
1	C	241[A]	LYS
1	C	266	LYS
1	C	267	GLU
1	C	268	ASN
1	D	105	MET
1	D	111	LYS
1	D	127	ARG
1	D	128	GLU
1	D	142[A]	SER
1	D	239	THR
1	D	241[A]	LYS
1	D	256	ARG
1	D	260	SER
1	D	266	LYS
1	D	267	GLU
1	D	268	ASN
1	E	110[A]	ARG
1	E	127	ARG
1	E	136	LYS
1	E	142[A]	SER
1	E	156	MET
1	E	165	ARG
1	E	214	LEU

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Mol	Chain	Res	Type
1	E	241[A]	LYS
1	E	247	THR
1	E	266	LYS
1	E	267	GLU
1	E	268	ASN
1	F	110[A]	ARG
1	F	128	GLU
1	F	142[A]	SER
1	F	153	ASN
1	F	154	THR
1	F	156	MET
1	F	165	ARG
1	F	172	HIS
1	F	214	LEU
1	F	241[A]	LYS
1	F	247	THR
1	F	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	211[A]	ASN
1	B	172	HIS
1	B	206	HIS
1	B	211[A]	ASN
1	C	206	HIS
1	C	211[A]	ASN
1	C	259	GLN
1	D	112	HIS
1	D	206	HIS
1	D	211[A]	ASN
1	D	259	GLN
1	E	139	GLN
1	E	206	HIS
1	E	211[A]	ASN
1	E	259	GLN
1	E	268	ASN
1	F	139	GLN
1	F	172	HIS
1	F	206	HIS
1	F	211[A]	ASN

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Mol	Chain	Res	Type
1	F	259	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	165/165 (100%)	-0.46	3 (1%)	68	68	13, 20, 40, 70	9 (5%)
1	B	165/165 (100%)	-0.48	3 (1%)	68	68	13, 20, 39, 72	8 (4%)
1	C	165/165 (100%)	-0.47	2 (1%)	79	79	12, 24, 40, 66	9 (5%)
1	D	165/165 (100%)	-0.48	1 (0%)	89	89	13, 23, 38, 50	9 (5%)
1	E	165/165 (100%)	-0.44	3 (1%)	68	68	17, 28, 41, 60	9 (5%)
1	F	165/165 (100%)	-0.42	2 (1%)	79	79	15, 28, 41, 55	9 (5%)
All	All	990/990 (100%)	-0.46	14 (1%)	75	76	12, 24, 40, 72	53 (5%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	ASN	6.8
1	A	268	ASN	6.0
1	E	156	MET	4.4
1	F	156	MET	4.4
1	F	155	GLY	3.2
1	A	267	GLU	3.2
1	C	268	ASN	2.9
1	A	266	LYS	2.8
1	B	266	LYS	2.7
1	C	156	MET	2.7
1	D	156	MET	2.4
1	E	154	THR	2.1
1	B	267	GLU	2.1
1	E	113	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	CA	F	929	1/1	0.97	0.09	35,35,35,35	0
2	ZN	D	916	1/1	0.98	0.07	24,24,24,24	0
2	ZN	E	921	1/1	0.98	0.09	22,22,22,22	0
2	ZN	E	922	1/1	0.98	0.07	35,35,35,35	0
2	ZN	F	927	1/1	0.98	0.07	35,35,35,35	0
3	CA	F	928	1/1	0.98	0.06	29,29,29,29	0
2	ZN	C	911	1/1	0.98	0.09	24,24,24,24	0
2	ZN	C	912	1/1	0.99	0.07	22,22,22,22	0
2	ZN	F	926	1/1	0.99	0.07	21,21,21,21	0
2	ZN	B	906	1/1	0.99	0.09	18,18,18,18	0
3	CA	A	903	1/1	0.99	0.07	16,16,16,16	0
3	CA	A	904	1/1	0.99	0.06	18,18,18,18	0
3	CA	B	908	1/1	0.99	0.08	15,15,15,15	0
3	CA	C	913	1/1	0.99	0.06	16,16,16,16	0
3	CA	C	914	1/1	0.99	0.03	21,21,21,21	0
3	CA	C	915	1/1	0.99	0.10	21,21,21,21	0
3	CA	D	918	1/1	0.99	0.07	17,17,17,17	0
3	CA	D	919	1/1	0.99	0.03	23,23,23,23	0
3	CA	D	920	1/1	0.99	0.07	22,22,22,22	0
3	CA	E	923	1/1	0.99	0.06	28,28,28,28	0
3	CA	E	924	1/1	0.99	0.07	35,35,35,35	0
3	CA	E	925	1/1	0.99	0.06	30,30,30,30	0
2	ZN	D	917	1/1	0.99	0.07	22,22,22,22	0
2	ZN	A	901	1/1	0.99	0.09	18,18,18,18	0
3	CA	F	930	1/1	0.99	0.06	30,30,30,30	0
2	ZN	A	902	1/1	1.00	0.09	18,18,18,18	0
3	CA	B	909	1/1	1.00	0.06	18,18,18,18	0
3	CA	B	910	1/1	1.00	0.07	16,16,16,16	0
2	ZN	B	907	1/1	1.00	0.09	17,17,17,17	0
3	CA	A	905	1/1	1.00	0.08	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.