



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:12 AM UTC

PDB ID : 9E2T / pdb\_00009e2t  
Title : Structure of a de novo designed interleukin-21 mimetic complex with IL-21R and IL-2Rg  
Authors : Abhiraman, G.C.; Jude, K.M.; Garcia, K.C.  
Deposited on : 2024-10-22  
Resolution : 2.28 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](mailto: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>.

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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

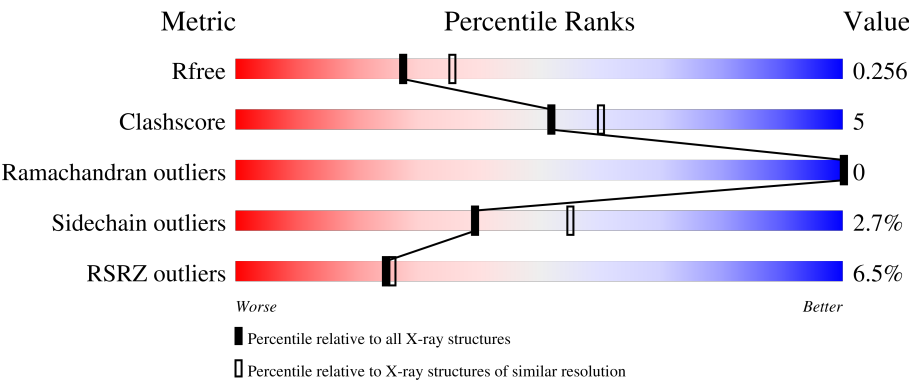
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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 <sub>free</sub>	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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  $\geq 3$ , 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	102	<div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>63%27%• 8%</div></div>
1	D	102	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>72%16%13%</div></div>
1	G	102	<div><div>22%</div><div><div></div><div></div><div></div><div></div></div><div>70%21%• 9%</div></div>
1	I	102	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>70%17%• 13%</div></div>
2	B	212	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>87%8%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	212	 4% 86% 13% .
2	H	212	 6% 80% 17% ..
2	J	212	 3% 91% 9%
3	C	203	 5% 83% 13% .
3	F	203	 3% 85% 12% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13255 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 21h10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	1	0
			778	480	145	147	6			
1	D	89	Total	C	N	O	S	0	0	0
			730	454	136	134	6			
1	G	93	Total	C	N	O	S	0	0	0
			762	471	141	144	6			
1	I	89	Total	C	N	O	S	0	0	0
			728	452	137	134	5			

- Molecule 2 is a protein called Interleukin-21 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	201	Total	C	N	O	S	0	0	0
			1621	1031	268	311	11			
2	E	210	Total	C	N	O	S	0	0	0
			1703	1081	279	332	11			
2	H	210	Total	C	N	O	S	0	1	0
			1709	1085	280	333	11			
2	J	212	Total	C	N	O	S	0	0	0
			1716	1088	281	336	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q9HBE5
B	-1	ASP	-	expression tag	UNP Q9HBE5
B	0	PRO	-	expression tag	UNP Q9HBE5
B	78	GLN	ASN	engineered mutation	UNP Q9HBE5
B	85	GLN	ASN	engineered mutation	UNP Q9HBE5
B	106	ASP	ASN	engineered mutation	UNP Q9HBE5
B	116	GLN	ASN	engineered mutation	UNP Q9HBE5
E	-2	ALA	-	expression tag	UNP Q9HBE5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASP	-	expression tag	UNP Q9HBE5
E	0	PRO	-	expression tag	UNP Q9HBE5
E	78	GLN	ASN	engineered mutation	UNP Q9HBE5
E	85	GLN	ASN	engineered mutation	UNP Q9HBE5
E	106	ASP	ASN	engineered mutation	UNP Q9HBE5
E	116	GLN	ASN	engineered mutation	UNP Q9HBE5
H	-2	ALA	-	expression tag	UNP Q9HBE5
H	-1	ASP	-	expression tag	UNP Q9HBE5
H	0	PRO	-	expression tag	UNP Q9HBE5
H	78	GLN	ASN	engineered mutation	UNP Q9HBE5
H	85	GLN	ASN	engineered mutation	UNP Q9HBE5
H	106	ASP	ASN	engineered mutation	UNP Q9HBE5
H	116	GLN	ASN	engineered mutation	UNP Q9HBE5
J	-2	ALA	-	expression tag	UNP Q9HBE5
J	-1	ASP	-	expression tag	UNP Q9HBE5
J	0	PRO	-	expression tag	UNP Q9HBE5
J	78	GLN	ASN	engineered mutation	UNP Q9HBE5
J	85	GLN	ASN	engineered mutation	UNP Q9HBE5
J	106	ASP	ASN	engineered mutation	UNP Q9HBE5
J	116	GLN	ASN	engineered mutation	UNP Q9HBE5

- Molecule 3 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1648	1048	291	301	8			
3	F	197	Total	C	N	O	S	0	0	0
			1667	1059	296	304	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	ALA	-	expression tag	UNP P31785
C	53	ASP	-	expression tag	UNP P31785
C	54	PRO	-	expression tag	UNP P31785
F	52	ALA	-	expression tag	UNP P31785
F	53	ASP	-	expression tag	UNP P31785
F	54	PRO	-	expression tag	UNP P31785

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	7	Total O 7 7	0	0
6	C	7	Total O 7 7	0	0
6	D	1	Total O 1 1	0	0

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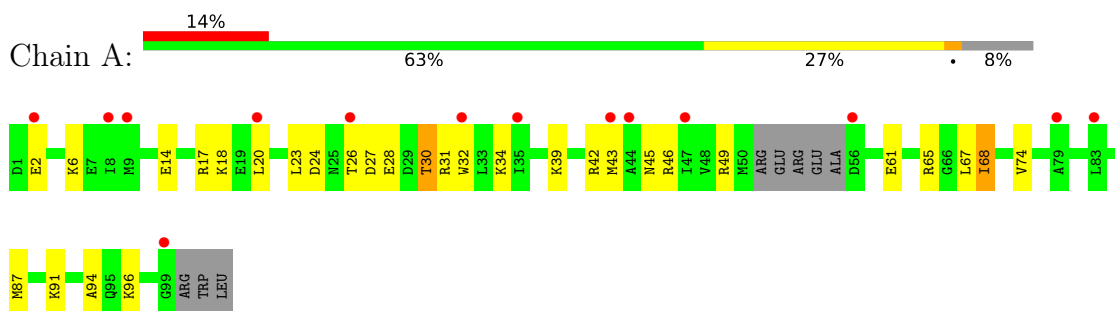
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total 4	O 4	0	0
6	F	3	Total 3	O 3	0	0
6	H	4	Total 4	O 4	0	0
6	J	5	Total 5	O 5	0	0



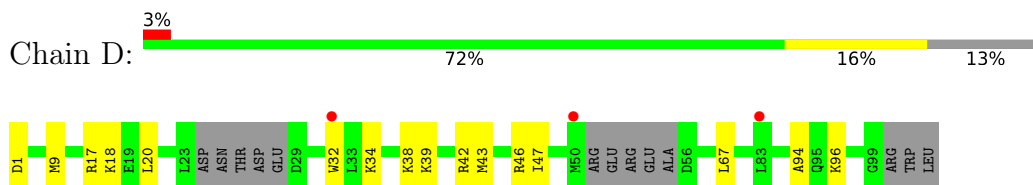
### 3 Residue-property plots [i](#)

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.

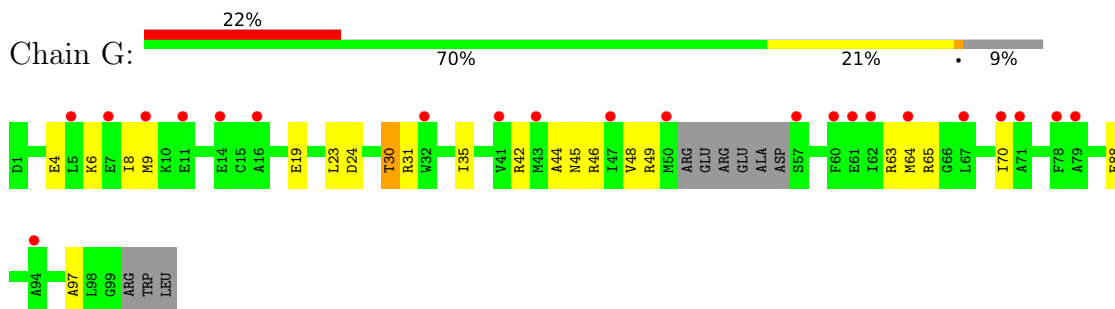
- Molecule 1: 21h10



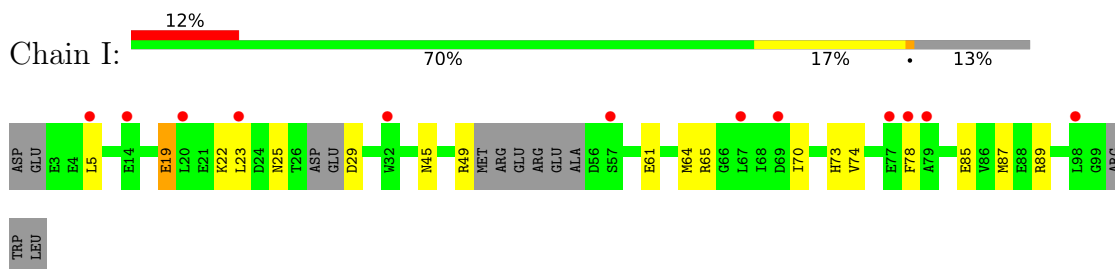
- Molecule 1: 21h10



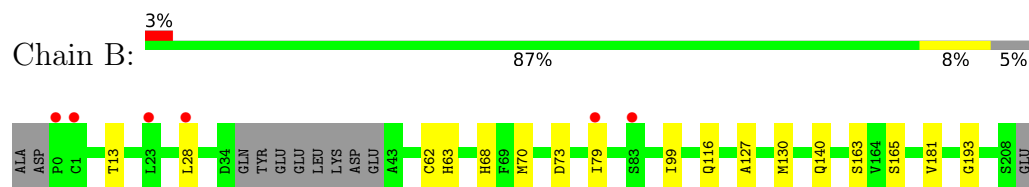
- Molecule 1: 21h10



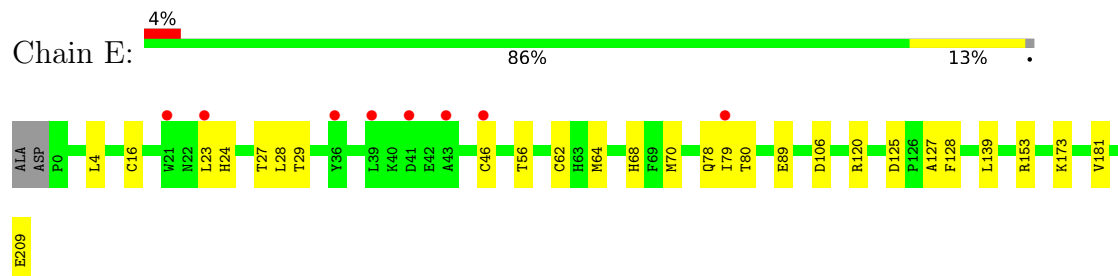
- Molecule 1: 21h10



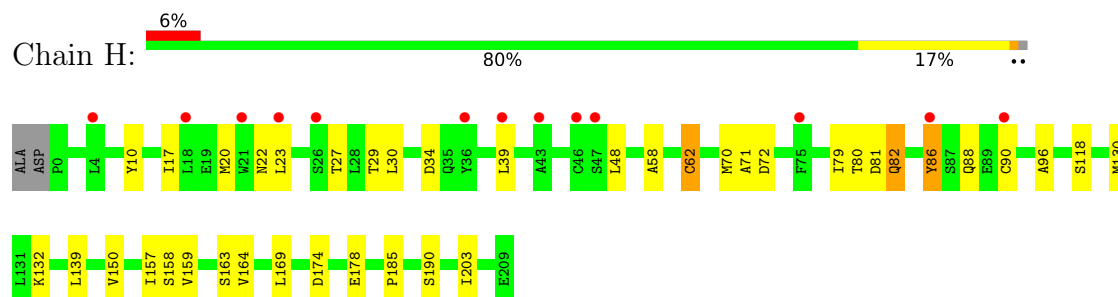
- Molecule 2: Interleukin-21 receptor



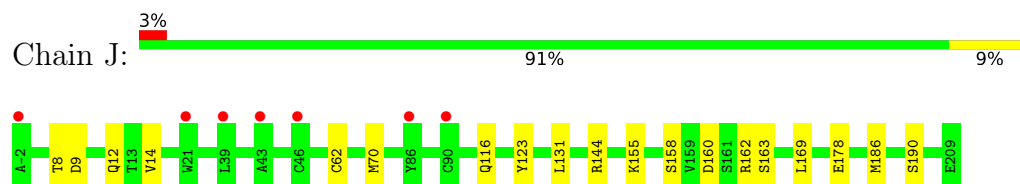
- Molecule 2: Interleukin-21 receptor



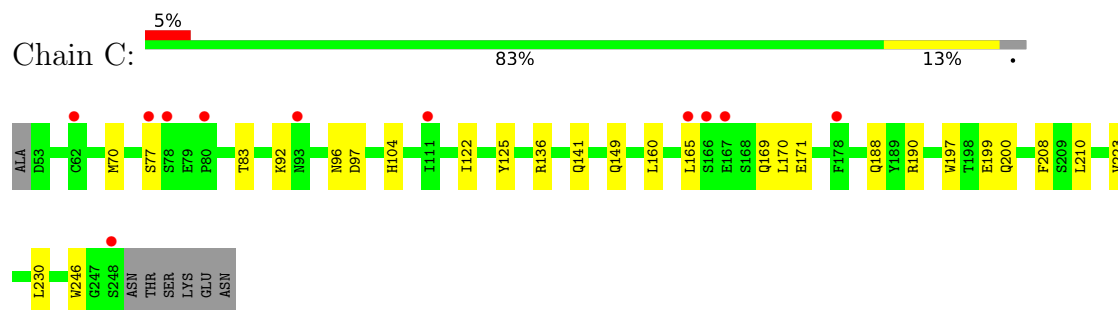
- Molecule 2: Interleukin-21 receptor



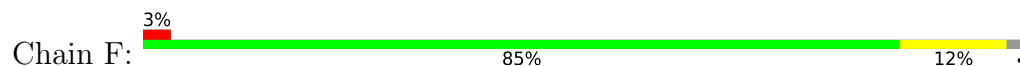
- Molecule 2: Interleukin-21 receptor

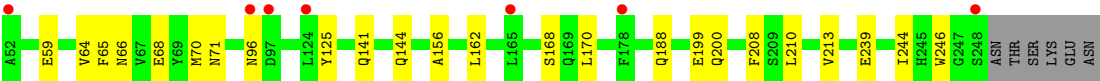


- Molecule 3: Cytokine receptor common subunit gamma



- Molecule 3: Cytokine receptor common subunit gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.50Å 78.08Å 101.22Å 94.63° 103.39° 114.55°	Depositor
Resolution (Å)	41.17 – 2.28 41.17 – 2.28	Depositor EDS
% Data completeness (in resolution range)	52.8 (41.17-2.28) 49.3 (41.17-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.199 , 0.242 0.218 , 0.256	Depositor DCC
$R_{free}$ test set	1934 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, EDO

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	0.20	0/784	0.32	0/1037
1	D	0.11	0/732	0.27	0/965
1	G	0.13	0/765	0.28	0/1012
1	I	0.11	0/730	0.25	0/964
2	B	0.13	0/1670	0.29	0/2276
2	E	0.13	0/1754	0.30	0/2390
2	H	0.13	0/1763	0.32	0/2402
2	J	0.13	0/1767	0.32	0/2409
3	C	0.13	0/1704	0.34	0/2325
3	F	0.12	0/1723	0.33	0/2348
All	All	0.13	0/13392	0.31	0/18128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	778	0	814	26	0
1	D	730	0	773	13	0
1	G	762	0	797	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	728	0	768	10	0
2	B	1621	0	1524	13	0
2	E	1703	0	1594	14	0
2	H	1709	0	1602	22	0
2	J	1716	0	1603	11	0
3	C	1648	0	1531	15	0
3	F	1667	0	1563	15	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
4	E	14	0	13	0	0
4	F	28	0	26	0	0
4	H	14	0	13	1	0
4	J	14	0	13	0	0
5	B	8	0	12	1	0
5	C	12	0	18	1	0
5	E	4	0	6	0	0
5	H	4	0	6	1	0
5	J	8	0	12	2	0
6	B	7	0	0	0	0
6	C	7	0	0	0	0
6	D	1	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
6	H	4	0	0	0	0
6	J	5	0	0	0	0
All	All	13255	0	12740	132	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 5.

All (132) 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)
2:H:157:ILE:HG12	2:H:164:VAL:HG11	1.67	0.77
2:H:20:MET:HE3	2:H:58:ALA:HB2	1.71	0.73
1:A:45:ASN:HB3	1:A:49:ARG:HH22	1.53	0.72
1:A:42[B]:ARG:NH2	2:B:68:HIS:O	2.25	0.70
1:A:28:GLU:O	1:A:31:ARG:HG2	1.91	0.69
1:A:96:LYS:HG2	3:C:125:TYR:HB3	1.74	0.68
1:I:45:ASN:HB3	1:I:49:ARG:HH22	1.59	0.67
1:G:63:ARG:NH1	2:H:72:ASP:OD2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HE2	2:B:70:MET:HG2	1.78	0.66
3:C:169:GLN:NE2	3:C:210:LEU:O	2.28	0.66
1:A:67:LEU:HD23	1:A:94:ALA:HB2	1.77	0.66
2:E:153:ARG:NH1	3:F:168:SER:OG	2.29	0.65
2:E:4:LEU:HD11	2:E:16:CYS:HB3	1.78	0.65
1:G:42:ARG:HB3	2:H:70:MET:HE1	1.79	0.65
2:E:106:ASP:OD2	2:E:120:ARG:NH1	2.30	0.64
2:J:116:GLN:NE2	2:J:163:SER:OG	2.30	0.64
3:F:156:ALA:HB2	3:F:239:GLU:HG2	1.82	0.60
3:C:160:LEU:HD21	3:C:223:VAL:HG23	1.82	0.60
1:I:74:VAL:HA	1:I:78:PHE:CD1	2.36	0.60
1:I:19:GLU:HA	1:I:22:LYS:HG2	1.83	0.60
2:B:28:LEU:HG	2:B:79:ILE:HG12	1.83	0.59
1:A:45:ASN:HB3	1:A:49:ARG:NH2	2.16	0.59
2:J:12:GLN:HB2	5:J:303:EDO:H11	1.85	0.58
2:J:144:ARG:HD2	2:J:178:GLU:HB2	1.85	0.58
2:H:27:THR:HB	2:H:80:THR:HB	1.87	0.57
2:E:173:LYS:HD3	2:E:209:GLU:HA	1.87	0.57
2:H:71:ALA:HB1	2:H:96:ALA:HB2	1.87	0.56
1:A:46:ARG:NH2	2:B:73:ASP:OD1	2.34	0.56
1:A:2:GLU:HB3	1:A:6:LYS:NZ	2.21	0.56
1:G:46:ARG:HA	1:G:49:ARG:NH2	2.20	0.56
1:D:17:ARG:HA	1:D:20:LEU:HD12	1.89	0.55
3:C:190:ARG:HD2	3:C:197:TRP:CE2	2.42	0.55
1:G:6:LYS:HG2	1:G:48:VAL:HA	1.89	0.55
2:H:79:ILE:HD13	2:H:90:CYS:HB2	1.89	0.54
2:H:185:PRO:HD2	5:H:302:EDO:H21	1.91	0.53
1:D:1:ASP:OD1	1:D:1:ASP:N	2.38	0.53
3:F:170:LEU:HB2	3:F:210:LEU:HD12	1.90	0.53
2:E:46:CYS:HB3	2:E:64:MET:HE2	1.90	0.53
3:F:200:GLN:HG2	3:F:208:PHE:CE1	2.45	0.52
1:A:43:MET:HG2	2:B:70:MET:SD	2.50	0.52
1:G:45:ASN:HB3	1:G:49:ARG:HH12	1.74	0.52
1:G:45:ASN:HB3	1:G:49:ARG:NH1	2.26	0.51
2:J:160:ASP:OD1	2:J:162:ARG:NH1	2.42	0.51
2:E:27:THR:HB	2:E:80:THR:HB	1.93	0.51
3:C:170:LEU:HB2	3:C:210:LEU:HD12	1.93	0.51
3:F:64:VAL:HG22	3:F:70:MET:HE2	1.92	0.51
1:G:19:GLU:O	1:G:23:LEU:HG	2.10	0.51
3:C:188:GLN:HG2	3:C:199:GLU:HG2	1.93	0.50
2:H:82:GLN:H	2:H:82:GLN:CD	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:OD1	1:A:28:GLU:N	2.42	0.50
1:I:45:ASN:HB3	1:I:49:ARG:NH2	2.26	0.50
2:B:116:GLN:OE1	2:B:165:SER:OG	2.29	0.50
3:C:200:GLN:HG2	3:C:208:PHE:CE1	2.47	0.49
1:D:42:ARG:HB2	2:E:70:MET:HE1	1.92	0.49
3:C:136:ARG:HD3	5:C:306:EDO:H12	1.95	0.49
3:F:162:LEU:HD23	3:F:170:LEU:HD13	1.95	0.49
2:J:9:ASP:OD2	5:J:303:EDO:O1	2.29	0.49
3:C:96:ASN:OD1	3:C:97:ASP:N	2.47	0.48
2:H:132:LYS:HG2	2:J:169:LEU:HD21	1.95	0.48
1:D:32:TRP:HB2	2:E:127:ALA:HB2	1.95	0.48
2:B:116:GLN:NE2	2:B:163:SER:OG	2.46	0.47
1:I:19:GLU:O	1:I:23:LEU:HG	2.14	0.47
1:A:45:ASN:HB3	1:A:49:ARG:HH12	1.79	0.47
1:A:45:ASN:CG	1:A:49:ARG:HH12	2.23	0.47
1:G:31:ARG:O	1:G:35:ILE:HG12	2.14	0.47
1:I:87:MET:HA	1:I:87:MET:HE2	1.97	0.47
1:A:42[A]:ARG:NH2	2:B:70:MET:HE2	2.30	0.47
1:D:96:LYS:HG2	3:F:125:TYR:HB3	1.95	0.46
3:C:83:THR:CB	3:C:136:ARG:HH12	2.27	0.46
1:A:45:ASN:CB	1:A:49:ARG:HH12	2.29	0.46
2:B:13:THR:HG22	2:B:63:HIS:ND1	2.30	0.46
1:D:42:ARG:O	1:D:46:ARG:HG3	2.16	0.46
1:A:32:TRP:HB2	2:B:127:ALA:HB2	1.98	0.46
2:B:99:ILE:O	2:B:193:GLY:HA3	2.16	0.46
3:C:165:LEU:HG	3:C:171:GLU:HB2	1.96	0.46
2:H:48:LEU:HG	2:H:62:CYS:HB3	1.98	0.46
2:B:140:GLN:HE21	5:B:303:EDO:H22	1.81	0.46
3:C:170:LEU:HD11	3:C:246:TRP:CE2	2.50	0.46
1:I:61:GLU:HG2	1:I:65:ARG:HD2	1.97	0.46
1:A:87:MET:HA	1:A:87:MET:HE2	1.97	0.46
2:H:34:ASP:CG	2:H:39:LEU:H	2.24	0.45
1:D:43:MET:HE3	1:D:43:MET:HB2	1.87	0.45
3:F:210:LEU:HD13	3:F:213:VAL:HG11	1.97	0.45
1:D:42:ARG:NH2	2:E:68:HIS:O	2.49	0.45
3:F:188:GLN:HG2	3:F:199:GLU:HG2	1.97	0.45
2:J:8:THR:HB	2:J:14:VAL:HG22	1.98	0.45
1:D:67:LEU:HD23	1:D:94:ALA:HB2	1.98	0.44
1:D:34:LYS:HE2	1:D:38:LYS:NZ	2.31	0.44
1:G:4:GLU:O	1:G:8:ILE:HG13	2.16	0.44
2:H:30:LEU:HD23	2:H:48:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:LEU:HG	2:H:157:ILE:HD11	2.00	0.44
2:E:28:LEU:HG	2:E:79:ILE:HG12	2.00	0.44
1:A:74:VAL:HG21	1:A:87:MET:HG3	1.99	0.44
2:E:139:LEU:HD12	2:E:181:VAL:HG13	1.99	0.44
1:G:65:ARG:HD3	2:H:190:SER:HB3	1.98	0.44
2:B:130:MET:HE2	2:B:130:MET:HB2	1.81	0.44
3:F:162:LEU:HD13	3:F:244:ILE:HD13	1.98	0.43
2:H:10:TYR:CE1	2:H:130:MET:HE3	2.53	0.43
2:H:17:ILE:HG21	4:H:301:NAG:H61	2.00	0.43
1:D:9:MET:HG3	1:D:47:ILE:HD12	2.01	0.43
1:G:9:MET:HB3	1:G:44:ALA:HA	1.99	0.43
1:A:68:ILE:HG23	1:A:91:LYS:HE3	2.00	0.43
1:D:39:LYS:HG2	2:E:70:MET:HE2	2.00	0.43
2:H:158:SER:OG	2:J:158:SER:OG	2.24	0.43
2:H:178:GLU:HG3	2:H:203:ILE:HG12	2.00	0.43
3:F:65:PHE:HE2	3:F:71:ASN:HB2	1.83	0.43
1:I:70:ILE:HA	1:I:73:HIS:HB3	2.01	0.43
1:A:61:GLU:HG2	1:A:65:ARG:HD2	2.00	0.43
2:E:78:GLN:HA	2:E:89:GLU:HA	2.00	0.43
1:I:5:LEU:HD22	1:I:64:MET:HE1	2.00	0.43
1:A:39:LYS:O	1:A:43:MET:HG3	2.18	0.43
3:C:92:LYS:HE2	3:C:92:LYS:HB3	1.82	0.43
3:F:170:LEU:HD11	3:F:246:TRP:CE2	2.54	0.43
2:H:86:TYR:C	2:H:86:TYR:CD1	2.98	0.42
3:F:66:ASN:O	3:F:68:GLU:HG3	2.19	0.42
3:C:70:MET:HE3	3:C:122:ILE:HG12	2.01	0.42
2:E:125:ASP:HB3	2:E:128:PHE:CD2	2.55	0.42
1:A:14:GLU:O	1:A:18:LYS:HD2	2.20	0.42
1:G:64:MET:HE2	1:G:97:ALA:HB3	2.01	0.41
2:J:123:TYR:CE1	2:J:131:LEU:HD12	2.55	0.41
1:A:23:LEU:HD21	1:A:30:THR:HA	2.02	0.41
3:F:59:GLU:HG3	3:F:144:GLN:HE22	1.85	0.41
1:A:45:ASN:HB3	1:A:49:ARG:NH1	2.35	0.41
1:A:17:ARG:HA	1:A:20:LEU:HD12	2.01	0.41
2:J:70:MET:HE3	2:J:70:MET:HB2	1.86	0.41
1:A:65:ARG:CZ	3:C:230:LEU:HD21	2.50	0.41
2:H:159:VAL:HG23	2:J:155:LYS:HD2	2.03	0.41
1:D:96:LYS:HE2	1:D:96:LYS:HB3	1.89	0.41
3:F:200:GLN:HG2	3:F:208:PHE:CZ	2.56	0.40
1:G:24:ASP:O	1:G:30:THR:OG1	2.36	0.40
2:H:22:ASN:OD1	2:H:23:LEU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:GLU:CD	1:I:89:ARG:HH12	2.29	0.40

There are no symmetry-related clashes.

## 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	91/102 (89%)	90 (99%)	1 (1%)	0	100	100
1	D	83/102 (81%)	83 (100%)	0	0	100	100
1	G	89/102 (87%)	89 (100%)	0	0	100	100
1	I	83/102 (81%)	83 (100%)	0	0	100	100
2	B	197/212 (93%)	188 (95%)	9 (5%)	0	100	100
2	E	208/212 (98%)	198 (95%)	10 (5%)	0	100	100
2	H	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
2	J	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
3	C	194/203 (96%)	182 (94%)	12 (6%)	0	100	100
3	F	195/203 (96%)	186 (95%)	9 (5%)	0	100	100
All	All	1559/1662 (94%)	1494 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	83/89 (93%)	78 (94%)	5 (6%)	17	23
1	D	77/89 (86%)	76 (99%)	1 (1%)	61	76
1	G	81/89 (91%)	78 (96%)	3 (4%)	30	43
1	I	77/89 (86%)	74 (96%)	3 (4%)	28	41
2	B	183/193 (95%)	181 (99%)	2 (1%)	65	79
2	E	192/193 (100%)	187 (97%)	5 (3%)	40	56
2	H	193/193 (100%)	182 (94%)	11 (6%)	18	25
2	J	193/193 (100%)	190 (98%)	3 (2%)	55	71
3	C	186/195 (95%)	182 (98%)	4 (2%)	45	62
3	F	189/195 (97%)	187 (99%)	2 (1%)	65	79
All	All	1454/1518 (96%)	1415 (97%)	39 (3%)	39	55

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	26	THR
1	A	30	THR
1	A	34	LYS
1	A	68	ILE
2	B	62	CYS
2	B	181	VAL
3	C	77	SER
3	C	104	HIS
3	C	141	GLN
3	C	149	GLN
1	D	18	LYS
2	E	23	LEU
2	E	24	HIS
2	E	29	THR
2	E	56	THR
2	E	62	CYS
3	F	96	ASN
3	F	141	GLN
1	G	30	THR
1	G	70	ILE
1	G	88	GLU
2	H	29	THR
2	H	62	CYS

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Mol	Chain	Res	Type
2	H	81	ASP
2	H	82	GLN
2	H	86	TYR
2	H	88	GLN
2	H	118	SER
2	H	150	VAL
2	H	163	SER
2	H	169	LEU
2	H	174	ASP
1	I	19	GLU
1	I	25	ASN
1	I	29	ASP
2	J	62	CYS
2	J	186	MET
2	J	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	95	GLN
3	C	118	GLN
3	C	141	GLN
3	C	149	GLN
3	C	216	GLN
2	E	49	HIS
3	F	96	ASN
3	F	126	GLN
3	F	141	GLN
3	F	144	GLN
2	H	49	HIS
2	J	33	GLN
2	J	53	HIS

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands 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	$\# Z  > 2$
5	EDO	B	302	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	J	303	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	J	302	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	C	305	-	3,3,3	0.44	0	2,2,2	0.34	0
4	NAG	C	301	3	14,14,15	0.43	0	17,19,21	0.61	1 (5%)
4	NAG	C	302	3	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	H	301	2	14,14,15	0.39	0	17,19,21	0.49	0
5	EDO	C	306	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	E	302	-	3,3,3	0.45	0	2,2,2	0.32	0
4	NAG	J	301	2	14,14,15	0.26	0	17,19,21	0.44	0
5	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.30	0
4	NAG	B	301	2	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	E	301	2	14,14,15	0.41	0	17,19,21	0.43	0
4	NAG	F	301	3	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
4	NAG	F	302	3	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	C	303	3	14,14,15	0.32	0	17,19,21	0.47	0
5	EDO	H	302	-	3,3,3	0.45	0	2,2,2	0.30	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
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	J	303	-	-	1/1/1/1	-
5	EDO	B	303	-	-	0/1/1/1	-
5	EDO	J	302	-	-	0/1/1/1	-
5	EDO	C	305	-	-	0/1/1/1	-
4	NAG	C	301	3	-	4/6/23/26	0/1/1/1
4	NAG	C	302	3	-	0/6/23/26	0/1/1/1
4	NAG	H	301	2	-	2/6/23/26	0/1/1/1
5	EDO	C	306	-	-	0/1/1/1	-
5	EDO	E	302	-	-	0/1/1/1	-
4	NAG	J	301	2	-	2/6/23/26	0/1/1/1
5	EDO	C	304	-	-	0/1/1/1	-
4	NAG	B	301	2	-	2/6/23/26	0/1/1/1
4	NAG	E	301	2	-	2/6/23/26	0/1/1/1
4	NAG	F	301	3	-	2/6/23/26	0/1/1/1
4	NAG	F	302	3	-	4/6/23/26	0/1/1/1
4	NAG	C	303	3	-	4/6/23/26	0/1/1/1
5	EDO	H	302	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	301	NAG	C1-O5-C5	2.32	115.30	112.19
4	C	301	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	NAG	O5-C5-C6-O6
4	H	301	NAG	C4-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6
4	F	301	NAG	O5-C5-C6-O6
4	C	303	NAG	C4-C5-C6-O6
4	H	301	NAG	O5-C5-C6-O6
4	E	301	NAG	O5-C5-C6-O6
4	B	301	NAG	C4-C5-C6-O6
4	C	301	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	301	NAG	O7-C7-N2-C2
4	C	303	NAG	C8-C7-N2-C2
4	C	303	NAG	O7-C7-N2-C2
4	F	302	NAG	C8-C7-N2-C2
4	F	302	NAG	O7-C7-N2-C2
4	E	301	NAG	C4-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
4	F	301	NAG	C4-C5-C6-O6
4	C	301	NAG	C4-C5-C6-O6
4	F	302	NAG	C4-C5-C6-O6
4	F	302	NAG	O5-C5-C6-O6
4	J	301	NAG	C4-C5-C6-O6
5	J	303	EDO	O1-C1-C2-O2
4	J	301	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	303	EDO	2	0
5	B	303	EDO	1	0
4	H	301	NAG	1	0
5	C	306	EDO	1	0
5	H	302	EDO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	94/102 (92%)	1.17	14 (14%) <b>5</b> <b>6</b>	41, 80, 141, 161	1 (1%)
1	D	89/102 (87%)	0.85	3 (3%) 48 50	39, 65, 97, 106	0
1	G	93/102 (91%)	1.52	22 (23%) <b>2</b> <b>2</b>	64, 93, 122, 142	0
1	I	89/102 (87%)	1.16	12 (13%) <b>7</b> <b>7</b>	57, 92, 121, 129	0
2	B	201/212 (94%)	0.37	6 (2%) 52 54	28, 47, 97, 129	0
2	E	210/212 (99%)	0.36	8 (3%) 44 46	25, 48, 98, 135	0
2	H	210/212 (99%)	0.52	13 (6%) <b>26</b> <b>27</b>	28, 50, 109, 142	1 (0%)
2	J	212/212 (100%)	0.45	7 (3%) 49 51	23, 48, 105, 142	0
3	C	196/203 (96%)	0.41	11 (5%) <b>30</b> <b>31</b>	28, 50, 98, 152	0
3	F	197/203 (97%)	0.34	7 (3%) 46 48	25, 46, 88, 149	0
All	All	1591/1662 (95%)	0.59	103 (6%) <b>25</b> <b>26</b>	23, 53, 110, 161	2 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	MET	5.2
2	J	21	TRP	5.0
1	I	78	PHE	4.7
1	G	5	LEU	4.5
1	G	78	PHE	4.3
2	B	23	LEU	4.2
2	E	23	LEU	3.7
1	G	67	LEU	3.6
1	I	23	LEU	3.5
2	H	90	CYS	3.5
1	G	64	MET	3.5
3	C	165	LEU	3.4
1	G	60	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	-2	ALA	3.4
2	E	21	TRP	3.4
1	A	43	MET	3.3
2	H	23	LEU	3.2
1	A	44	ALA	3.2
2	H	39	LEU	3.2
1	I	67	LEU	3.2
1	G	47	ILE	3.2
2	H	43	ALA	3.1
3	C	248	SER	3.0
1	I	5	LEU	3.0
1	A	2	GLU	3.0
1	A	99	GLY	2.9
1	G	79	ALA	2.9
2	H	21	TRP	2.9
2	E	36	TYR	2.9
3	C	93	ASN	2.8
1	I	77	GLU	2.8
1	I	14	GLU	2.8
3	C	78	SER	2.7
2	J	46	CYS	2.7
3	C	62	CYS	2.7
2	H	36	TYR	2.7
2	H	46	CYS	2.7
2	J	39	LEU	2.7
1	G	16	ALA	2.7
1	A	32	TRP	2.7
3	C	178	PHE	2.6
1	G	70	ILE	2.6
3	F	248	SER	2.6
1	A	26	THR	2.6
1	A	47	ILE	2.6
2	B	1	CYS	2.5
1	G	57	SER	2.5
1	A	35	ILE	2.5
2	B	28	LEU	2.5
1	A	9	MET	2.5
1	D	32	TRP	2.4
1	A	20	LEU	2.4
1	G	43	MET	2.4
1	I	69	ASP	2.4
2	E	41	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	96	ASN	2.4
3	F	97	ASP	2.4
1	A	79	ALA	2.4
1	I	79	ALA	2.4
2	B	79	ILE	2.4
3	C	167	GLU	2.4
3	F	178	PHE	2.3
1	A	8	ILE	2.3
3	C	111	ILE	2.3
1	G	61	GLU	2.3
2	H	18	LEU	2.3
2	B	0	PRO	2.3
3	C	80	PRO	2.3
1	G	50	MET	2.3
1	I	20	LEU	2.3
2	H	4	LEU	2.3
3	F	124	LEU	2.3
1	G	71	ALA	2.3
2	J	43	ALA	2.3
2	B	83	SER	2.3
1	D	50	MET	2.2
2	H	26	SER	2.2
2	E	79	ILE	2.2
1	I	98	LEU	2.2
2	E	39	LEU	2.2
1	G	11	GLU	2.2
1	G	14	GLU	2.2
1	G	94	ALA	2.2
3	C	166	SER	2.2
1	I	32	TRP	2.2
1	A	83	LEU	2.2
2	J	86	TYR	2.2
1	D	83	LEU	2.2
1	G	62	ILE	2.2
2	H	47	SER	2.2
3	C	77	SER	2.2
2	H	86	TYR	2.1
2	H	75	PHE	2.1
3	F	52	ALA	2.1
3	F	165	LEU	2.1
1	A	56	ASP	2.1
1	G	41	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	32	TRP	2.1
2	J	90	CYS	2.1
1	G	7	GLU	2.1
2	E	43	ALA	2.0
2	E	46	CYS	2.0
1	I	57	SER	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	EDO	C	306	4/4	0.58	0.20	69,75,84,87	0
4	NAG	C	302	14/15	0.78	0.11	77,91,100,100	0
5	EDO	J	303	4/4	0.81	0.17	44,51,54,61	0
4	NAG	C	303	14/15	0.82	0.11	53,62,74,76	0
5	EDO	C	304	4/4	0.83	0.14	52,63,64,68	0
4	NAG	C	301	14/15	0.84	0.10	46,59,68,71	0
4	NAG	E	301	14/15	0.85	0.09	49,57,69,69	0
4	NAG	B	301	14/15	0.85	0.10	50,58,63,64	0
4	NAG	H	301	14/15	0.86	0.10	60,67,75,76	0
4	NAG	F	301	14/15	0.86	0.11	35,43,60,73	0
4	NAG	J	301	14/15	0.87	0.10	44,55,67,68	0
5	EDO	B	303	4/4	0.88	0.12	32,37,46,56	0
5	EDO	E	302	4/4	0.88	0.12	38,38,54,59	0
5	EDO	C	305	4/4	0.88	0.14	42,49,50,54	0
5	EDO	J	302	4/4	0.90	0.11	38,41,44,50	0
5	EDO	B	302	4/4	0.90	0.09	27,30,32,59	0
4	NAG	F	302	14/15	0.91	0.07	49,57,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	H	302	4/4	0.92	0.10	40,47,50,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.