



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:02 PM GMT

PDB ID : 1N7Z
Title : Structure and location of gene product 8 in the bacteriophage T4 baseplate
Authors : Leiman, P.G.; Shneider, M.M.; Kostyuchenko, V.A.; Chipman, P.R.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2002-11-18
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

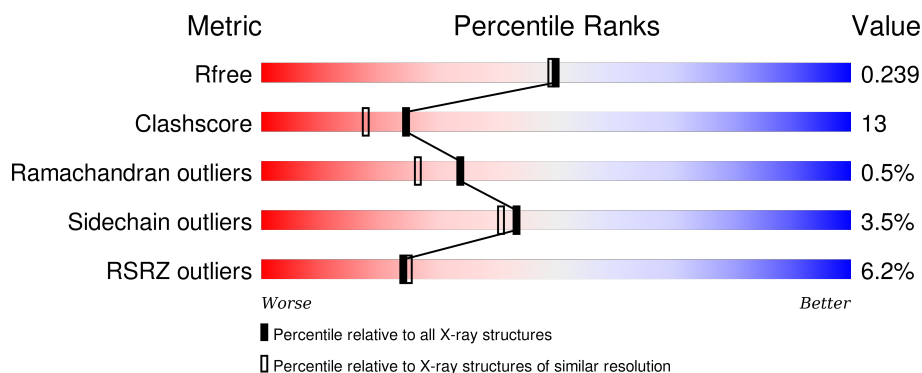
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	334	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	334	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	334	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	334	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>

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
2	CL	A	1703	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11579 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 baseplate structural protein gp8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	0	0
			2631	1677	430	507	5	12			
1	B	328	Total	C	N	O	S	Se	0	0	0
			2631	1677	430	507	5	12			
1	C	328	Total	C	N	O	S	Se	0	0	0
			2631	1677	430	507	5	12			
1	D	328	Total	C	N	O	S	Se	0	0	0
			2631	1677	430	507	5	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	71	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	75	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	76	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	85	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	141	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	167	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	303	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	309	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	312	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	320	MSE	MET	MODIFIED RESIDUE	UNP P19062
A	322	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	21	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	71	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	75	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	76	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	85	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	141	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	167	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	303	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	309	MSE	MET	MODIFIED RESIDUE	UNP P19062

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Chain	Residue	Modelled	Actual	Comment	Reference
B	312	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	320	MSE	MET	MODIFIED RESIDUE	UNP P19062
B	322	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	21	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	71	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	75	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	76	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	85	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	141	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	167	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	303	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	309	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	312	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	320	MSE	MET	MODIFIED RESIDUE	UNP P19062
C	322	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	21	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	71	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	75	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	76	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	85	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	141	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	167	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	303	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	309	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	312	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	320	MSE	MET	MODIFIED RESIDUE	UNP P19062
D	322	MSE	MET	MODIFIED RESIDUE	UNP P19062

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	6	Total Cl 6 6	0	0
2	A	9	Total Cl 9 9	0	0
2	D	6	Total Cl 6 6	0	0
2	C	9	Total Cl 9 9	0	0

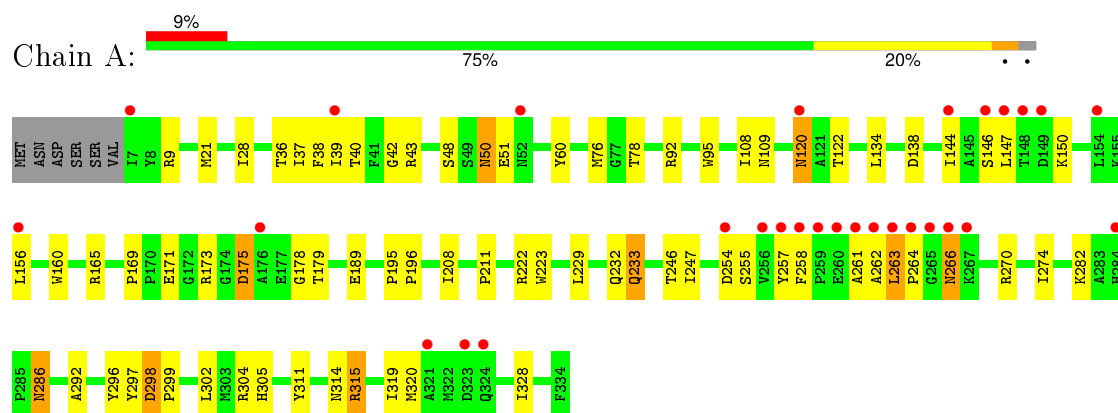
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	279	Total 279	O 279	0	0
3	C	234	Total 234	O 234	0	0
3	D	268	Total 268	O 268	0	0

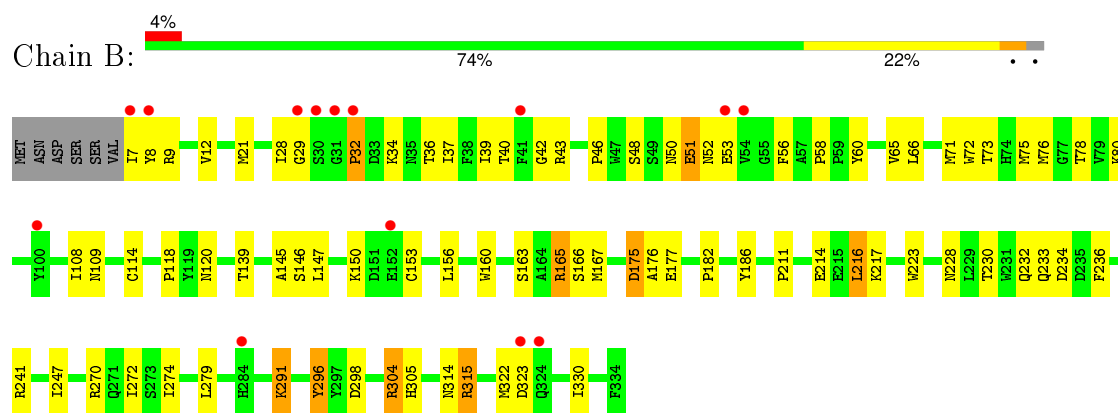
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

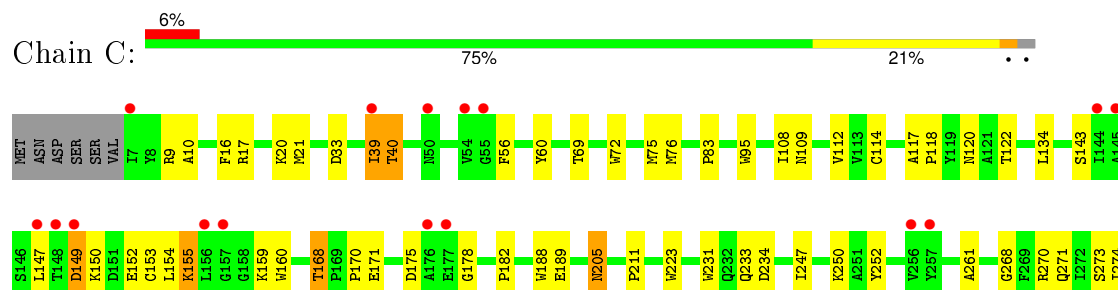
- Molecule 1: baseplate structural protein gp8

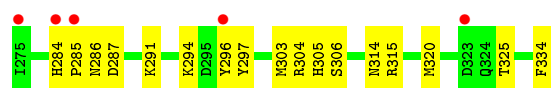


- Molecule 1: baseplate structural protein gp8

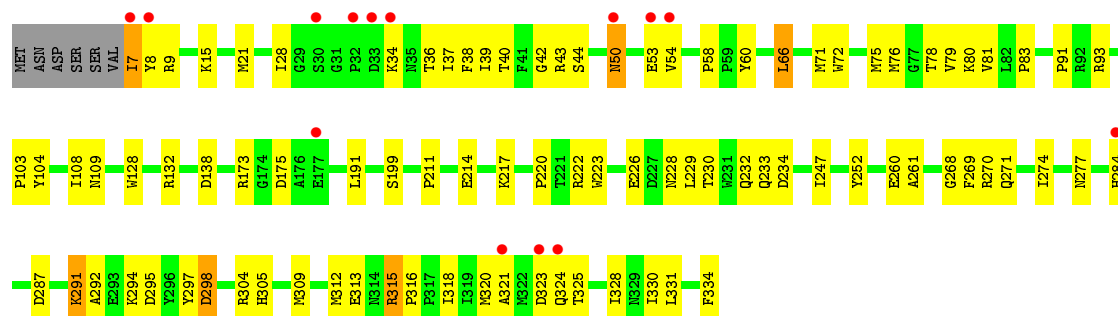


- Molecule 1: baseplate structural protein gp8





- Molecule 1: baseplate structural protein gp8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.39Å 78.47Å 88.23Å 110.96° 97.60° 111.39°	Depositor
Resolution (Å)	27.08 – 2.00 27.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (27.08-2.00) 81.8 (27.08-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.240 0.212 , 0.239	Depositor DCC
R_{free} test set	2410 reflections (2.48%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97291 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11579	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:
CL

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	0.34	0/2697	0.62	0/3658
1	B	0.37	0/2697	0.65	1/3658 (0.0%)
1	C	0.34	0/2697	0.61	0/3658
1	D	0.36	0/2697	0.63	1/3658 (0.0%)
All	All	0.35	0/10788	0.63	2/14632 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	ASP	N-CA-C	-5.60	95.88	111.00
1	B	298	ASP	N-CA-C	-5.39	96.44	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2631	0	2509	68	0
1	B	2631	0	2509	73	0
1	C	2631	0	2509	69	0
1	D	2631	0	2509	74	0
2	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	1	0
2	C	9	0	0	2	0
2	D	6	0	0	2	0
3	A	244	0	0	12	0
3	B	279	0	0	7	0
3	C	234	0	0	11	0
3	D	268	0	0	11	0
All	All	11579	0	10036	266	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 13.

All (266) 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:D:228:ASN:HD21	1:D:230:THR:HG22	1.17	1.05
1:A:95:TRP:HB3	1:A:120:ASN:HD21	1.21	1.02
1:B:28:ILE:HD11	1:B:37:ILE:HD12	1.44	0.98
1:A:266:ASN:HB3	1:A:319:ILE:HG23	1.51	0.91
1:D:217:LYS:HA	3:D:1925:HOH:O	1.72	0.88
1:D:220:PRO:HG3	3:D:1925:HOH:O	1.75	0.85
1:D:228:ASN:ND2	1:D:230:THR:HG22	1.92	0.83
1:B:228:ASN:HD21	1:B:230:THR:HG22	1.44	0.81
1:D:83:PRO:HG2	2:D:1726:CL:CL	2.18	0.81
1:C:205:ASN:HD22	1:C:205:ASN:H	1.28	0.78
1:B:147:LEU:HD21	1:B:156:LEU:HD12	1.68	0.74
1:D:315:ARG:HB2	1:D:316:PRO:HD2	1.69	0.74
1:A:254:ASP:O	3:A:1873:HOH:O	2.06	0.73
1:A:40:THR:HG22	1:A:78:THR:HG22	1.70	0.72
3:A:1831:HOH:O	1:B:232:GLN:HG2	1.90	0.71
1:A:222:ARG:HH21	1:A:222:ARG:HG2	1.56	0.71
1:A:286:ASN:HA	3:A:1925:HOH:O	1.91	0.71
1:D:229:LEU:O	1:D:232:GLN:HG3	1.92	0.70
1:B:28:ILE:HD11	1:B:37:ILE:CD1	2.22	0.69
1:A:255:SER:C	3:A:1873:HOH:O	2.32	0.68
1:D:291:LYS:HD3	3:D:1837:HOH:O	1.92	0.68
1:A:258:PHE:CD1	3:A:1873:HOH:O	2.47	0.68
1:A:258:PHE:HD2	1:A:261:ALA:HB3	1.59	0.68
1:C:10:ALA:HB2	1:D:313:GLU:HG3	1.76	0.68
1:D:228:ASN:HD21	1:D:230:THR:CG2	2.00	0.67
1:B:40:THR:HG22	1:B:78:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD11	1:A:156:LEU:HD12	1.75	0.67
1:D:7:ILE:N	1:D:7:ILE:HD13	2.10	0.67
1:A:282:LYS:NZ	3:A:1831:HOH:O	2.27	0.66
1:A:95:TRP:HB3	1:A:120:ASN:ND2	2.04	0.66
1:B:228:ASN:ND2	1:B:230:THR:HG22	2.10	0.66
1:B:71:MSE:HE1	3:B:1774:HOH:O	1.94	0.65
1:B:279:LEU:HD21	1:B:291:LYS:HE2	1.78	0.65
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.61	0.65
3:C:1909:HOH:O	1:D:316:PRO:HG2	1.95	0.65
1:B:228:ASN:HD21	1:B:230:THR:CG2	2.10	0.65
1:C:56:PHE:O	1:D:7:ILE:HD11	1.96	0.63
1:B:36:THR:HG23	1:B:80:LYS:HE3	1.81	0.63
1:D:39:ILE:HG22	1:D:79:VAL:HG22	1.80	0.63
1:A:175:ASP:HB2	1:A:179:THR:H	1.64	0.63
3:A:1925:HOH:O	1:B:232:GLN:HG2	1.98	0.62
1:B:51:GLU:HA	1:B:56:PHE:CD1	2.35	0.62
1:A:262:ALA:HA	1:A:266:ASN:ND2	2.15	0.62
1:B:51:GLU:HA	1:B:56:PHE:CG	2.35	0.62
1:B:322:MSE:HE3	1:B:323:ASP:OD2	1.98	0.62
1:D:40:THR:HG22	1:D:78:THR:HG22	1.82	0.61
1:B:28:ILE:HG22	1:B:29:GLY:N	2.15	0.61
1:A:9:ARG:HD2	1:B:58:PRO:O	2.01	0.61
1:A:257:TYR:N	3:A:1873:HOH:O	2.34	0.60
1:A:262:ALA:HA	1:A:266:ASN:HD21	1.66	0.60
1:B:72:TRP:HB3	1:B:304:ARG:HD2	1.84	0.60
1:C:60:TYR:CE1	1:D:9:ARG:HD2	2.37	0.59
1:C:16:PHE:CE1	1:C:20:LYS:HE3	2.37	0.59
1:C:205:ASN:N	1:C:205:ASN:HD22	2.00	0.59
1:A:50:ASN:HD22	1:A:50:ASN:N	2.00	0.59
1:A:39:ILE:HD11	1:A:328:ILE:HG21	1.85	0.59
1:D:321:ALA:O	1:D:324:GLN:HB3	2.02	0.58
1:B:165:ARG:HD2	1:B:167:MSE:SE	2.52	0.58
1:B:66:LEU:HD12	3:B:1789:HOH:O	2.04	0.58
1:D:43:ARG:NE	3:D:1914:HOH:O	2.36	0.58
1:C:152:GLU:HA	1:C:155:LYS:HG2	1.86	0.58
1:A:108:ILE:O	1:A:109:ASN:HB2	2.04	0.57
1:B:234:ASP:OD1	1:B:241:ARG:HD2	2.05	0.57
1:C:39:ILE:HD13	1:C:274:ILE:HD11	1.85	0.57
1:B:43:ARG:HG2	1:B:270:ARG:HB2	1.86	0.57
1:C:147:LEU:HD13	1:C:153:CYS:HA	1.86	0.57
1:C:304:ARG:NH1	3:C:1774:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:CYS:SG	1:C:170:PRO:HD2	2.45	0.57
1:C:315:ARG:HB3	1:D:8:TYR:CD1	2.40	0.56
1:D:324:GLN:HG2	1:D:325:THR:N	2.20	0.56
1:D:39:ILE:CG2	1:D:79:VAL:HG22	2.35	0.56
1:D:173:ARG:HH22	1:D:226:GLU:CD	2.09	0.56
1:D:21:MSE:HG3	1:D:247:ILE:HG13	1.88	0.56
1:D:309:MSE:SE	1:D:312:MSE:HE3	2.56	0.56
1:A:222:ARG:HG2	1:A:222:ARG:NH2	2.19	0.55
1:B:50:ASN:O	1:B:53:GLU:HG2	2.06	0.55
1:C:69:THR:HA	1:C:305:HIS:HE1	1.71	0.55
1:C:315:ARG:HB3	1:D:8:TYR:CE1	2.41	0.55
1:A:50:ASN:HD22	1:A:50:ASN:H	1.53	0.55
1:D:72:TRP:HA	1:D:75:MSE:HE3	1.89	0.55
1:B:39:ILE:HA	1:B:274:ILE:HD13	1.88	0.54
1:B:72:TRP:HA	1:B:75:MSE:HE3	1.90	0.54
1:C:170:PRO:HG3	1:C:188:TRP:CD1	2.42	0.54
1:C:20:LYS:HE2	1:D:334:PHE:CD1	2.42	0.54
1:D:42:GLY:C	1:D:76:MSE:HE2	2.28	0.54
1:B:165:ARG:HD3	1:B:166:SER:O	2.08	0.54
1:C:294:LYS:HB2	1:C:297:TYR:CZ	2.44	0.53
1:C:21:MSE:HG3	1:C:247:ILE:HG13	1.89	0.53
1:B:108:ILE:O	1:B:109:ASN:HB2	2.08	0.53
1:A:258:PHE:CD2	1:A:261:ALA:HB3	2.42	0.53
1:A:42:GLY:HA2	1:A:76:MSE:HG3	1.91	0.53
1:A:315:ARG:HB3	1:B:8:TYR:CE1	2.43	0.53
1:B:114:CYS:HA	1:B:120:ASN:OD1	2.09	0.53
1:C:108:ILE:O	1:C:109:ASN:HB2	2.09	0.52
1:B:21:MSE:HG3	1:B:247:ILE:HG13	1.91	0.52
1:C:304:ARG:HG3	3:C:1774:HOH:O	2.09	0.52
1:A:266:ASN:CB	1:A:319:ILE:HG23	2.33	0.52
1:A:258:PHE:CE2	1:A:320:MSE:SE	3.13	0.52
1:D:277:ASN:OD1	1:D:291:LYS:NZ	2.33	0.52
1:B:50:ASN:O	1:B:52:ASN:N	2.43	0.51
1:D:28:ILE:HD12	1:D:37:ILE:HG23	1.92	0.51
1:C:149:ASP:OD2	1:C:149:ASP:N	2.41	0.51
1:A:258:PHE:N	3:A:1873:HOH:O	2.05	0.51
1:D:34:LYS:NZ	3:D:1992:HOH:O	2.40	0.51
1:B:270:ARG:HH11	1:B:270:ARG:HG3	1.75	0.51
1:A:144:ILE:O	1:A:144:ILE:HG22	2.10	0.50
1:D:108:ILE:O	1:D:109:ASN:HB2	2.12	0.50
1:B:147:LEU:HD12	1:B:147:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD23	1:B:153:CYS:HA	1.92	0.50
1:D:53:GLU:HG2	1:D:54:VAL:N	2.27	0.50
3:C:1909:HOH:O	1:D:318:ILE:HD11	2.11	0.50
1:A:134:LEU:HD11	1:A:189:GLU:HB2	1.93	0.50
1:C:76:MSE:HE3	1:C:261:ALA:HB2	1.94	0.50
1:B:304:ARG:NH1	3:B:1770:HOH:O	2.38	0.49
1:C:297:TYR:N	3:C:1932:HOH:O	2.45	0.49
1:C:134:LEU:HD11	1:C:189:GLU:HB2	1.94	0.49
1:D:36:THR:HG22	1:D:38:PHE:CE1	2.48	0.49
1:A:292:ALA:HB1	1:A:297:TYR:CE2	2.47	0.49
1:D:39:ILE:HG22	1:D:79:VAL:CG2	2.42	0.49
1:C:69:THR:HA	1:C:305:HIS:CE1	2.47	0.49
1:C:117:ALA:HB1	1:C:118:PRO:HD2	1.94	0.49
1:D:268:GLY:HA2	3:D:1916:HOH:O	2.12	0.49
1:A:178:GLY:O	1:A:189:GLU:HA	2.12	0.49
1:C:9:ARG:HD3	1:D:60:TYR:CD1	2.47	0.49
1:C:122:THR:HB	1:C:171:GLU:HG2	1.93	0.49
1:D:294:LYS:HG2	1:D:297:TYR:OH	2.13	0.49
1:C:320:MSE:HG2	3:C:1778:HOH:O	2.12	0.49
1:C:40:THR:HG23	1:C:75:MSE:HG3	1.94	0.48
1:C:40:THR:HG21	1:C:75:MSE:HE2	1.95	0.48
1:C:120:ASN:O	1:C:122:THR:HG23	2.13	0.48
1:B:182:PRO:HD2	1:B:186:TYR:O	2.13	0.48
1:A:263:LEU:HD12	1:A:264:PRO:HD3	1.95	0.48
1:D:39:ILE:HD11	1:D:328:ILE:HG21	1.96	0.48
1:A:315:ARG:HB3	1:B:8:TYR:CD1	2.48	0.48
1:B:139:THR:HG22	1:B:163:SER:OG	2.14	0.47
1:A:9:ARG:HD3	1:B:60:TYR:CD1	2.49	0.47
1:B:52:ASN:HB2	3:B:1896:HOH:O	2.13	0.47
1:A:122:THR:HB	1:A:171:GLU:HB3	1.95	0.47
1:C:303:MSE:HG3	1:C:306:SER:HB3	1.96	0.47
1:C:291:LYS:HB3	1:C:291:LYS:NZ	2.29	0.47
1:B:314:ASN:C	1:B:315:ARG:HG2	2.35	0.47
1:A:263:LEU:HD12	1:A:264:PRO:CD	2.45	0.47
1:C:271:GLN:HG2	1:C:314:ASN:OD1	2.13	0.47
1:B:48:SER:O	1:B:51:GLU:HG2	2.14	0.47
1:C:168:THR:HG23	1:C:182:PRO:HB3	1.97	0.47
1:A:21:MSE:HG3	1:A:247:ILE:HG13	1.96	0.47
1:C:143:SER:HB2	1:C:159:LYS:H	1.80	0.46
1:B:279:LEU:CD2	1:B:291:LYS:HE2	2.43	0.46
1:B:12:VAL:HG23	1:B:12:VAL:O	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ILE:HD12	1:C:154:LEU:HD21	1.97	0.46
1:B:330:ILE:HG12	3:B:1902:HOH:O	2.15	0.46
1:A:229:LEU:O	1:A:232:GLN:HG3	2.16	0.46
1:A:286:ASN:ND2	3:A:1925:HOH:O	2.31	0.46
1:C:285:PRO:HG2	3:C:1927:HOH:O	2.16	0.46
1:B:42:GLY:HA2	1:B:76:MSE:HE3	1.98	0.46
1:D:128:TRP:CE2	1:D:199:SER:HB2	2.51	0.46
1:B:214:GLU:HG2	2:B:1710:CL:CL	2.53	0.46
1:C:178:GLY:O	1:C:189:GLU:HA	2.16	0.46
1:A:92:ARG:HB2	1:A:208:ILE:HG23	1.98	0.46
1:B:211:PRO:HB3	1:B:223:TRP:CE2	2.50	0.46
1:B:118:PRO:C	1:B:120:ASN:H	2.19	0.45
1:C:76:MSE:HE3	1:C:261:ALA:CB	2.45	0.45
1:C:250:LYS:NZ	2:C:1718:CL:CL	2.86	0.45
1:A:28:ILE:HG12	1:A:37:ILE:HD12	1.98	0.45
1:B:230:THR:HG23	1:B:234:ASP:OD1	2.17	0.45
1:D:40:THR:CG2	1:D:78:THR:HG22	2.47	0.45
1:C:72:TRP:HA	1:C:75:MSE:HE3	1.98	0.45
1:B:73:THR:OG1	3:B:1770:HOH:O	2.21	0.45
1:D:291:LYS:HG3	1:D:291:LYS:O	2.17	0.45
1:B:71:MSE:HG2	3:B:1768:HOH:O	2.16	0.45
1:A:60:TYR:HA	1:B:9:ARG:HB3	1.99	0.45
1:C:296:TYR:HB2	3:C:1932:HOH:O	2.17	0.45
1:D:44:SER:HA	1:D:268:GLY:O	2.17	0.45
1:B:32:PRO:HD3	3:D:1887:HOH:O	2.16	0.45
1:B:28:ILE:HG22	1:B:29:GLY:H	1.80	0.44
1:C:69:THR:HG23	3:C:1870:HOH:O	2.16	0.44
1:B:304:ARG:HG3	1:B:305:HIS:CD2	2.53	0.44
1:C:143:SER:CB	1:C:159:LYS:H	2.31	0.44
1:B:147:LEU:CD2	1:B:153:CYS:HA	2.48	0.44
1:D:270:ARG:HG3	1:D:270:ARG:HH11	1.82	0.44
1:D:211:PRO:HB3	1:D:223:TRP:CE2	2.52	0.44
1:D:230:THR:HG23	1:D:234:ASP:OD1	2.18	0.44
1:C:9:ARG:HD2	1:D:58:PRO:O	2.17	0.44
1:D:284:HIS:HB2	1:D:287:ASP:OD2	2.18	0.44
1:D:175:ASP:HB2	3:D:1838:HOH:O	2.18	0.44
1:C:10:ALA:HB2	1:D:313:GLU:CG	2.47	0.44
1:C:304:ARG:NH1	1:C:304:ARG:HG3	2.30	0.44
1:A:36:THR:HG22	1:A:38:PHE:CE1	2.53	0.44
1:C:17:ARG:HD2	1:C:334:PHE:O	2.17	0.44
3:A:1891:HOH:O	1:B:32:PRO:HG3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:GLU:HG2	1:D:54:VAL:H	1.82	0.43
1:D:330:ILE:HG22	1:D:331:LEU:N	2.33	0.43
1:D:132:ARG:HB2	1:D:191:LEU:HD11	2.00	0.43
1:C:231:TRP:HA	1:C:234:ASP:OD2	2.17	0.43
1:A:39:ILE:O	1:A:39:ILE:HG23	2.18	0.43
1:B:46:PRO:HA	1:B:270:ARG:NE	2.33	0.43
1:A:195:PRO:HA	1:A:196:PRO:HD3	1.89	0.43
1:D:15:LYS:HE3	3:D:1957:HOH:O	2.17	0.43
1:C:286:ASN:HB2	3:C:1927:HOH:O	2.19	0.43
1:B:175:ASP:OD2	1:B:176:ALA:N	2.45	0.43
1:D:71:MSE:HE1	1:D:271:GLN:HB3	2.01	0.43
1:B:36:THR:CG2	1:B:80:LYS:HE3	2.48	0.43
1:C:268:GLY:HA2	3:C:1778:HOH:O	2.18	0.43
1:B:217:LYS:HG2	1:B:236:PHE:CD2	2.54	0.43
1:A:120:ASN:HA	1:A:120:ASN:HD22	1.56	0.43
1:C:60:TYR:CZ	1:D:9:ARG:HD2	2.54	0.42
1:B:65:VAL:HG23	1:B:66:LEU:N	2.34	0.42
1:D:261:ALA:O	1:D:320:MSE:HE3	2.19	0.42
1:B:150:LYS:HA	1:B:160:TRP:CE3	2.54	0.42
1:A:297:TYR:CG	1:A:302:LEU:HD21	2.54	0.42
1:D:214:GLU:HB2	2:D:1724:CL:CL	2.56	0.42
1:D:37:ILE:CG1	1:D:81:VAL:HB	2.50	0.42
1:B:150:LYS:HG3	1:B:160:TRP:CG	2.54	0.42
1:A:150:LYS:HG3	1:A:160:TRP:CD1	2.54	0.42
1:C:83:PRO:HD2	2:C:1719:CL:CL	2.56	0.42
1:D:50:ASN:HD21	1:D:53:GLU:CB	2.32	0.42
1:C:95:TRP:HB3	1:C:120:ASN:OD1	2.19	0.42
1:A:36:THR:CG2	1:A:38:PHE:CE1	3.03	0.42
1:C:252:TYR:HB3	1:C:325:THR:CG2	2.50	0.42
1:B:40:THR:O	1:B:272:ILE:HA	2.20	0.42
1:A:211:PRO:HB3	1:A:223:TRP:CE2	2.55	0.42
1:C:33:ASP:N	1:C:33:ASP:OD2	2.53	0.42
1:D:304:ARG:HG2	1:D:305:HIS:CD2	2.55	0.42
1:B:296:TYR:OH	1:D:295:ASP:HB2	2.20	0.42
1:D:91:PRO:HG2	3:D:1781:HOH:O	2.18	0.42
1:A:50:ASN:H	1:A:50:ASN:ND2	2.18	0.42
1:A:314:ASN:C	1:A:315:ARG:HG3	2.38	0.42
1:D:36:THR:HG23	1:D:80:LYS:HD2	2.02	0.42
1:A:233:GLN:HB2	1:A:233:GLN:HE21	1.72	0.42
1:A:274:ILE:HB	1:A:311:TYR:HB3	2.02	0.42
1:A:173:ARG:O	1:A:178:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HD11	1:A:37:ILE:HD12	2.01	0.41
1:A:255:SER:HA	1:A:258:PHE:CZ	2.55	0.41
1:A:28:ILE:CD1	1:A:37:ILE:HD12	2.50	0.41
1:B:270:ARG:HG3	1:B:270:ARG:NH1	2.33	0.41
1:D:66:LEU:HD13	3:D:1886:HOH:O	2.19	0.41
1:C:170:PRO:HG3	1:C:188:TRP:CG	2.55	0.41
1:B:114:CYS:HA	1:B:120:ASN:CG	2.40	0.41
1:A:9:ARG:HD3	1:B:60:TYR:CE1	2.56	0.41
1:C:95:TRP:O	1:C:120:ASN:OD1	2.39	0.41
1:D:269:PHE:HE1	1:D:315:ARG:HH21	1.68	0.41
1:C:39:ILE:CD1	1:C:274:ILE:HD11	2.50	0.41
1:A:304:ARG:HG2	1:A:305:HIS:CD2	2.55	0.41
1:C:270:ARG:HG3	1:C:270:ARG:HH11	1.85	0.41
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.85	0.41
1:D:103:PRO:HG2	1:D:104:TYR:CD2	2.56	0.41
1:A:43:ARG:HG2	1:A:270:ARG:HB2	2.01	0.41
1:C:150:LYS:HG3	1:C:160:TRP:CG	2.55	0.41
1:A:286:ASN:HD22	1:A:286:ASN:HA	1.61	0.41
1:C:16:PHE:CZ	1:C:20:LYS:HE3	2.55	0.41
1:D:252:TYR:HB3	1:D:325:THR:CG2	2.51	0.41
1:D:43:ARG:N	1:D:76:MSE:HE2	2.36	0.41
1:C:315:ARG:HD2	1:D:8:TYR:CE1	2.56	0.41
1:A:138:ASP:HA	1:A:150:LYS:HE3	2.02	0.41
1:A:298:ASP:O	1:A:299:PRO:C	2.59	0.41
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.93	0.41
1:A:48:SER:O	1:A:51:GLU:HB2	2.21	0.41
1:A:95:TRP:CH2	1:A:169:PRO:HD3	2.56	0.40
1:D:292:ALA:HB1	1:D:297:TYR:CE2	2.57	0.40
3:A:1891:HOH:O	1:B:34:LYS:HE2	2.21	0.40
1:C:233:GLN:HB2	1:C:233:GLN:HE21	1.70	0.40
1:C:211:PRO:HB3	1:C:223:TRP:CE2	2.55	0.40
1:B:12:VAL:CG2	1:B:12:VAL:O	2.69	0.40
1:A:296:TYR:CG	1:A:297:TYR:N	2.89	0.40
1:C:284:HIS:N	1:C:287:ASP:OD2	2.53	0.40
1:D:39:ILE:HA	1:D:274:ILE:HD13	2.03	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	326/334 (98%)	311 (95%)	13 (4%)	2 (1%)	30	22
1	B	326/334 (98%)	311 (95%)	11 (3%)	4 (1%)	16	8
1	C	326/334 (98%)	315 (97%)	11 (3%)	0	100	100
1	D	326/334 (98%)	317 (97%)	9 (3%)	0	100	100
All	All	1304/1336 (98%)	1254 (96%)	44 (3%)	6 (0%)	34	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	GLU
1	B	145	ALA
1	B	175	ASP
1	A	175	ASP
1	B	32	PRO
1	A	146	SER

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	289/283 (102%)	279 (96%)	10 (4%)	43	40
1	B	289/283 (102%)	279 (96%)	10 (4%)	43	40
1	C	289/283 (102%)	280 (97%)	9 (3%)	47	46
1	D	289/283 (102%)	277 (96%)	12 (4%)	36	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1156/1132 (102%)	1115 (96%)	41 (4%)	43 40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	120	ASN
1	A	165	ARG
1	A	233	GLN
1	A	246	THR
1	A	263	LEU
1	A	266	ASN
1	A	286	ASN
1	A	298	ASP
1	A	315	ARG
1	B	7	ILE
1	B	146	SER
1	B	165	ARG
1	B	177	GLU
1	B	216	LEU
1	B	233	GLN
1	B	291	LYS
1	B	296	TYR
1	B	304	ARG
1	B	315	ARG
1	C	39	ILE
1	C	40	THR
1	C	112	VAL
1	C	149	ASP
1	C	155	LYS
1	C	168	THR
1	C	175	ASP
1	C	205	ASN
1	C	273	SER
1	D	7	ILE
1	D	50	ASN
1	D	66	LEU
1	D	93	ARG
1	D	138	ASP
1	D	222	ARG
1	D	233	GLN
1	D	260	GLU

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Mol	Chain	Res	Type
1	D	291	LYS
1	D	298	ASP
1	D	315	ARG
1	D	323	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	50	ASN
1	A	52	ASN
1	A	120	ASN
1	A	232	GLN
1	A	233	GLN
1	A	266	ASN
1	A	286	ASN
1	A	305	HIS
1	A	324	GLN
1	A	329	ASN
1	B	233	GLN
1	B	277	ASN
1	B	286	ASN
1	B	329	ASN
1	C	23	ASN
1	C	205	ASN
1	C	233	GLN
1	C	271	GLN
1	C	286	ASN
1	C	305	HIS
1	D	23	ASN
1	D	50	ASN
1	D	52	ASN
1	D	228	ASN
1	D	232	GLN
1	D	233	GLN
1	D	329	ASN

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 carbohydrates 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 ⓘ

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	316/334 (94%)	0.36	29 (9%) 11 12	14, 30, 59, 69	0
1	B	316/334 (94%)	0.09	14 (4%) 38 39	14, 27, 43, 57	0
1	C	316/334 (94%)	0.21	21 (6%) 22 22	15, 31, 53, 57	0
1	D	316/334 (94%)	0.10	14 (4%) 38 39	14, 28, 46, 64	0
All	All	1264/1336 (94%)	0.19	78 (6%) 24 25	14, 29, 52, 69	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	PRO	8.3
1	D	323	ASP	7.7
1	B	31	GLY	7.4
1	A	262	ALA	6.0
1	D	33	ASP	5.8
1	D	32	PRO	5.0
1	A	321	ALA	5.0
1	A	264	PRO	4.9
1	C	144	ILE	4.9
1	A	259	PRO	4.7
1	A	257	TYR	4.5
1	A	261	ALA	4.3
1	A	323	ASP	4.3
1	D	324	GLN	4.2
1	C	176	ALA	4.0
1	A	260	GLU	4.0
1	C	145	ALA	3.9
1	B	324	GLN	3.8
1	D	7	ILE	3.6
1	C	7	ILE	3.6
1	A	256	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	30	SER	3.5
1	A	156	LEU	3.5
1	A	265	GLY	3.4
1	D	8	TYR	3.4
1	B	323	ASP	3.3
1	A	258	PHE	3.3
1	A	176	ALA	3.2
1	C	323	ASP	3.2
1	C	147	LEU	3.1
1	A	148	THR	3.1
1	A	266	ASN	3.1
1	C	296	TYR	3.1
1	A	7	ILE	3.1
1	D	54	VAL	3.1
1	C	157	GLY	3.1
1	A	144	ILE	3.0
1	D	53	GLU	3.0
1	C	257	TYR	3.0
1	A	263	LEU	3.0
1	C	149	ASP	2.9
1	D	30	SER	2.9
1	A	154	LEU	2.8
1	A	284	HIS	2.8
1	B	284	HIS	2.7
1	B	8	TYR	2.7
1	C	50	ASN	2.6
1	A	267	LYS	2.6
1	A	147	LEU	2.5
1	C	275	ILE	2.5
1	A	149	ASP	2.5
1	C	148	THR	2.5
1	B	29	GLY	2.5
1	C	285	PRO	2.4
1	B	54	VAL	2.4
1	C	256	VAL	2.4
1	A	146	SER	2.4
1	C	284	HIS	2.4
1	C	55	GLY	2.4
1	C	54	VAL	2.3
1	D	50	ASN	2.3
1	A	39	ILE	2.2
1	C	156	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	152	GLU	2.2
1	D	177	GLU	2.2
1	A	324	GLN	2.2
1	A	254	ASP	2.2
1	C	39	ILE	2.1
1	D	34	LYS	2.1
1	B	41	PHE	2.1
1	C	177	GLU	2.1
1	D	321	ALA	2.1
1	B	7	ILE	2.1
1	A	52	ASN	2.1
1	D	284	HIS	2.0
1	B	53	GLU	2.0
1	A	120	ASN	2.0
1	B	100	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	CL	A	1703	1/1	0.98	0.18	4.67	33,33,33,33	0
2	CL	D	1728	1/1	0.92	0.10	-0.07	53,53,53,53	0
2	CL	C	1716	1/1	0.99	0.05	-0.84	25,25,25,25	0
2	CL	D	1724	1/1	0.99	0.09	-0.84	33,33,33,33	0
2	CL	B	1710	1/1	0.98	0.07	-1.39	44,44,44,44	0
2	CL	C	1721	1/1	0.94	0.06	-1.62	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	C	1717	1/1	0.97	0.05	-2.58	35,35,35,35	0
2	CL	A	1729	1/1	0.98	0.06	-2.61	37,37,37,37	0
2	CL	B	1709	1/1	0.99	0.09	-	33,33,33,33	0
2	CL	D	1727	1/1	0.97	0.06	-	39,39,39,39	0
2	CL	A	1706	1/1	0.97	0.12	-	34,34,34,34	0
2	CL	B	1714	1/1	0.81	0.13	-	55,55,55,55	0
2	CL	A	1705	1/1	0.97	0.07	-	43,43,43,43	0
2	CL	C	1718	1/1	0.93	0.06	-	43,43,43,43	0
2	CL	D	1725	1/1	0.96	0.06	-	37,37,37,37	0
2	CL	A	1708	1/1	0.88	0.11	-	57,57,57,57	0
2	CL	A	1702	1/1	0.99	0.10	-	26,26,26,26	0
2	CL	C	1730	1/1	0.95	0.09	-	38,38,38,38	0
2	CL	A	1701	1/1	0.99	0.04	-	27,27,27,27	0
2	CL	D	1723	1/1	0.98	0.06	-	28,28,28,28	0
2	CL	C	1720	1/1	0.96	0.09	-	44,44,44,44	0
2	CL	D	1726	1/1	0.93	0.11	-	38,38,38,38	0
2	CL	B	1711	1/1	0.93	0.10	-	42,42,42,42	0
2	CL	C	1715	1/1	0.98	0.05	-	28,28,28,28	0
2	CL	C	1722	1/1	0.95	0.24	-	57,57,57,57	0
2	CL	A	1704	1/1	0.97	0.10	-	41,41,41,41	0
2	CL	B	1713	1/1	0.95	0.09	-	41,41,41,41	0
2	CL	C	1719	1/1	0.97	0.05	-	40,40,40,40	0
2	CL	A	1707	1/1	0.97	0.10	-	46,46,46,46	0
2	CL	B	1712	1/1	0.98	0.06	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.