Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 02:05 PM EDT

PDB ID	:	4RHB
Title	:	Crystal structure of the lipopolysaccharide assembly complex LptD-LptE from the Escherichia coli outer membrane
Authors	:	Malojcic, G.; Garner, R.A.; Kahne, D.
Deposited on	:	2014-10-01
Resolution	:	3.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

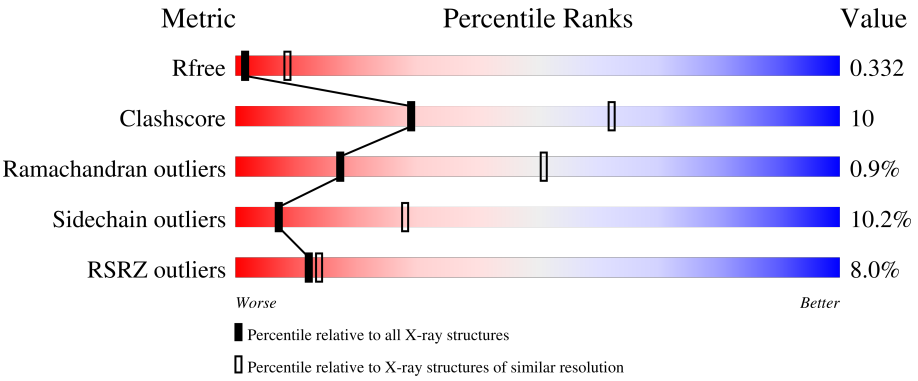
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	614	7% 67% 20% • 9%
1	C	614	7% 67% 20% • 9%
2	B	175	5% 65% 20% • 14%
2	D	175	9% 63% 21% • 14%

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
4	NA	B	201	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11615 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	6	0
			4618	2917	780	907	14			
1	C	557	Total	C	N	O	S	0	6	0
			4626	2923	781	908	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	MET	-	expression tag	UNP P31554
A	180	LYS	-	expression tag	UNP P31554
A	181	LYS	-	expression tag	UNP P31554
A	182	ARG	-	expression tag	UNP P31554
A	183	ILE	-	expression tag	UNP P31554
A	184	PRO	-	expression tag	UNP P31554
A	185	THR	-	expression tag	UNP P31554
A	186	LEU	-	expression tag	UNP P31554
A	187	LEU	-	expression tag	UNP P31554
A	188	ALA	-	expression tag	UNP P31554
A	189	THR	-	expression tag	UNP P31554
A	190	MET	-	expression tag	UNP P31554
A	191	ILE	-	expression tag	UNP P31554
A	192	ALA	-	expression tag	UNP P31554
A	193	THR	-	expression tag	UNP P31554
A	194	ALA	-	expression tag	UNP P31554
A	195	LEU	-	expression tag	UNP P31554
A	196	TYR	-	expression tag	UNP P31554
A	197	SER	-	expression tag	UNP P31554
A	198	GLN	-	expression tag	UNP P31554
A	199	GLN	-	expression tag	UNP P31554
A	200	GLY	-	expression tag	UNP P31554
A	201	LEU	-	expression tag	UNP P31554
A	202	ALA	-	expression tag	UNP P31554
A	785	HIS	-	expression tag	UNP P31554

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Chain	Residue	Modelled	Actual	Comment	Reference
A	786	HIS	-	expression tag	UNP P31554
A	787	HIS	-	expression tag	UNP P31554
A	788	HIS	-	expression tag	UNP P31554
A	789	HIS	-	expression tag	UNP P31554
A	790	HIS	-	expression tag	UNP P31554
A	791	HIS	-	expression tag	UNP P31554
A	792	HIS	-	expression tag	UNP P31554
C	179	MET	-	expression tag	UNP P31554
C	180	LYS	-	expression tag	UNP P31554
C	181	LYS	-	expression tag	UNP P31554
C	182	ARG	-	expression tag	UNP P31554
C	183	ILE	-	expression tag	UNP P31554
C	184	PRO	-	expression tag	UNP P31554
C	185	THR	-	expression tag	UNP P31554
C	186	LEU	-	expression tag	UNP P31554
C	187	LEU	-	expression tag	UNP P31554
C	188	ALA	-	expression tag	UNP P31554
C	189	THR	-	expression tag	UNP P31554
C	190	MET	-	expression tag	UNP P31554
C	191	ILE	-	expression tag	UNP P31554
C	192	ALA	-	expression tag	UNP P31554
C	193	THR	-	expression tag	UNP P31554
C	194	ALA	-	expression tag	UNP P31554
C	195	LEU	-	expression tag	UNP P31554
C	196	TYR	-	expression tag	UNP P31554
C	197	SER	-	expression tag	UNP P31554
C	198	GLN	-	expression tag	UNP P31554
C	199	GLN	-	expression tag	UNP P31554
C	200	GLY	-	expression tag	UNP P31554
C	201	LEU	-	expression tag	UNP P31554
C	202	ALA	-	expression tag	UNP P31554
C	785	HIS	-	expression tag	UNP P31554
C	786	HIS	-	expression tag	UNP P31554
C	787	HIS	-	expression tag	UNP P31554
C	788	HIS	-	expression tag	UNP P31554
C	789	HIS	-	expression tag	UNP P31554
C	790	HIS	-	expression tag	UNP P31554
C	791	HIS	-	expression tag	UNP P31554
C	792	HIS	-	expression tag	UNP P31554

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1181	737	215	222	7			
2	D	150	Total	C	N	O	S	0	0	0
			1181	737	215	222	7			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

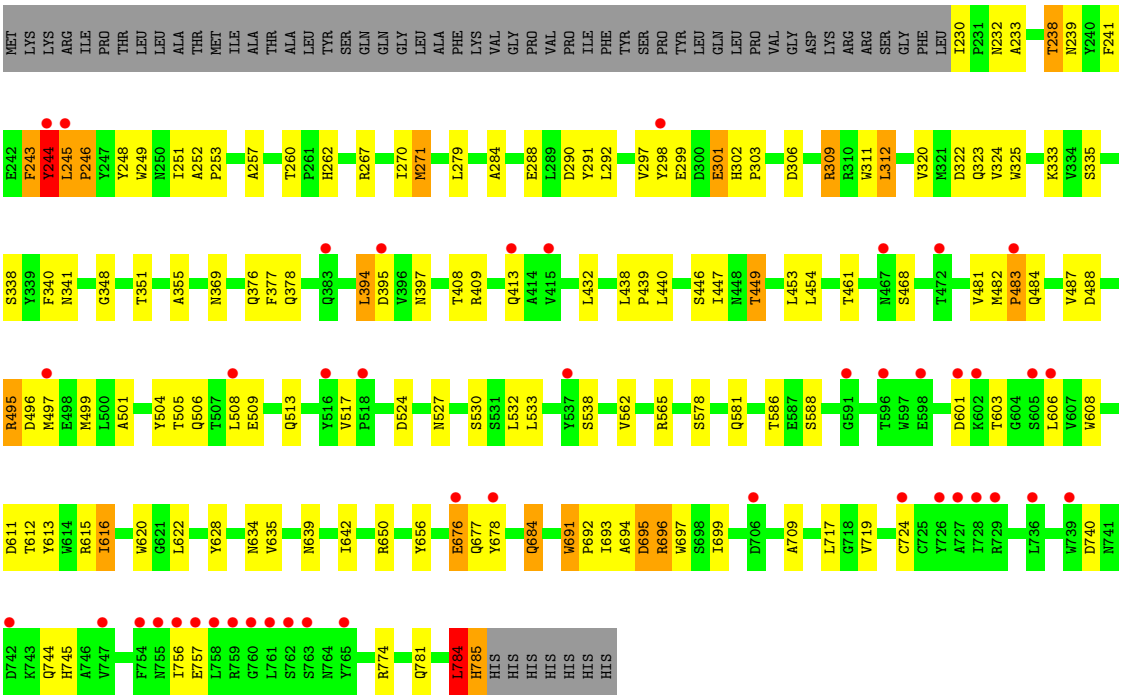
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	C	3	Total	O	0	0
			3	3		

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.

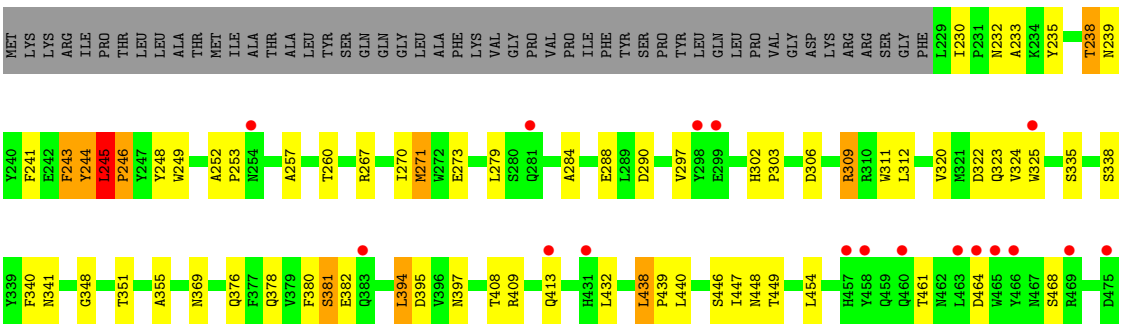
• Molecule 1: LPS-assembly protein LptD

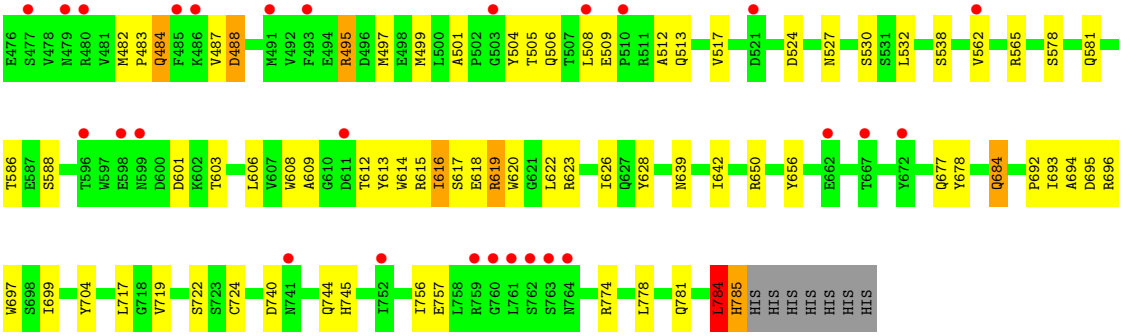
Chain A:



• Molecule 1: LPS-assembly protein LptD

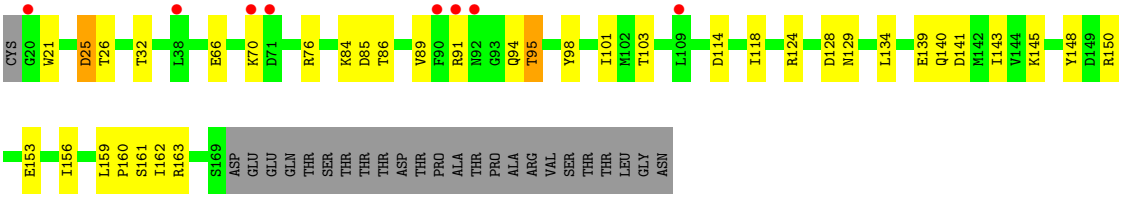
Chain C:





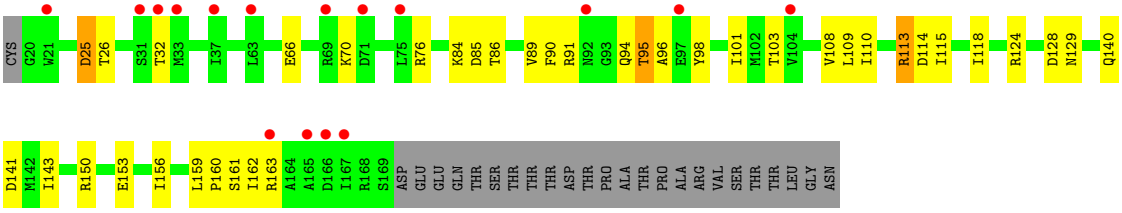
• Molecule 2: LPS-assembly lipoprotein LptE

Chain B:



• Molecule 2: LPS-assembly lipoprotein LptE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.04Å 136.62Å 108.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.31 – 3.35 108.31 – 3.36	Depositor EDS
% Data completeness (in resolution range)	96.3 (108.31-3.35) 96.3 (108.31-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.257 , 0.338 0.258 , 0.332	Depositor DCC
R_{free} test set	1250 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	96.2	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11615	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.56	1/4756 (0.0%)	0.77	5/6477 (0.1%)
1	C	0.53	0/4764	0.75	1/6488 (0.0%)
2	B	0.48	0/1198	0.69	0/1617
2	D	0.48	0/1198	0.71	0/1617
All	All	0.53	1/11916 (0.0%)	0.75	6/16199 (0.0%)

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	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	TRP	CB-CG	6.46	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	LEU	N-CA-C	-8.89	87.00	111.00
1	A	244[A]	TYR	N-CA-C	6.99	129.86	111.00
1	A	244[B]	TYR	N-CA-C	6.99	129.86	111.00
1	C	245	LEU	CA-CB-CG	6.96	131.31	115.30
1	A	691	TRP	CA-CB-CG	6.03	125.16	113.70
1	A	245	LEU	N-CA-CB	5.94	122.28	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244[A]	TYR	Peptide
1	A	244[B]	TYR	Peptide
1	C	784	LEU	Peptide

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	4618	0	4274	88	0
1	C	4626	0	4285	87	0
2	B	1181	0	1212	23	0
2	D	1181	0	1212	33	0
3	A	1	0	0	0	0
3	C	3	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	1	0
All	All	11615	0	10983	216	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 10.

All (216) 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:D:108:VAL:O	2:D:115:ILE:CD1	1.73	1.34
2:D:108:VAL:O	2:D:115:ILE:HD11	1.08	1.23
1:C:235[B]:TYR:CE1	1:C:241[B]:PHE:CD1	2.29	1.21
1:C:235[B]:TYR:CE1	1:C:241[B]:PHE:HD1	1.58	1.21
1:A:297:VAL:O	1:A:301:GLU:OE1	1.59	1.20
1:C:235[B]:TYR:HE1	1:C:241[B]:PHE:CD1	1.63	1.08
2:D:108:VAL:O	2:D:115:ILE:CG1	2.04	1.04
1:C:235[B]:TYR:HE1	1:C:241[B]:PHE:CE1	1.75	1.03
1:C:784:LEU:HG	1:C:785:HIS:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:O	1:A:301:GLU:CD	1.99	1.00
2:B:86:THR:HG23	2:B:95:THR:HG23	1.50	0.94
2:D:86:THR:HG23	2:D:95:THR:HG23	1.51	0.91
2:D:108:VAL:C	2:D:115:ILE:HD11	1.94	0.86
2:D:109:LEU:HA	2:D:115:ILE:HG12	1.61	0.82
2:D:109:LEU:HA	2:D:115:ILE:CD1	2.10	0.82
1:C:781:GLN:HG2	5:C:901:HOH:O	1.79	0.81
2:D:109:LEU:HA	2:D:115:ILE:CG1	2.12	0.79
1:A:495:ARG:HG2	2:B:21:TRP:CZ3	2.23	0.74
1:C:616:ILE:HD13	1:C:620:TRP:HB3	1.72	0.72
1:A:239:ASN:OD1	1:A:267:ARG:NE	2.22	0.71
1:C:239:ASN:OD1	1:C:267:ARG:NE	2.24	0.71
1:A:351:THR:HG21	2:B:86:THR:HG21	1.75	0.69
1:A:453:LEU:HD11	1:A:481:VAL:CG1	2.24	0.68
1:C:351:THR:HG21	2:D:86:THR:HG21	1.74	0.67
1:C:623:ARG:HH21	1:C:784:LEU:HD22	1.59	0.67
1:C:484:GLN:HB2	1:C:517:VAL:HG22	1.76	0.67
1:A:484:GLN:HB2	1:A:517:VAL:HG22	1.76	0.66
1:C:696:ARG:HG3	1:C:722:SER:O	1.96	0.65
1:C:235[B]:TYR:CD1	1:C:241[B]:PHE:HD1	2.12	0.65
1:A:298:TYR:HA	1:A:301:GLU:OE2	1.97	0.64
1:C:235[B]:TYR:CE1	1:C:241[B]:PHE:CE1	2.67	0.64
1:C:623:ARG:NH2	1:C:784:LEU:HD22	2.13	0.64
1:C:614:TRP:CE2	1:C:616:ILE:HG23	2.33	0.63
1:A:355:ALA:HB3	1:A:378:GLN:HB3	1.82	0.62
2:D:109:LEU:HA	2:D:115:ILE:HD13	1.79	0.62
1:A:301:GLU:CD	1:A:301:GLU:N	2.53	0.62
1:A:249:TRP:HB3	1:A:257:ALA:HB3	1.81	0.61
1:C:249:TRP:HB3	1:C:257:ALA:HB3	1.82	0.61
1:C:355:ALA:HB3	1:C:378:GLN:HB3	1.82	0.61
1:C:603:THR:O	1:C:606:LEU:HD21	2.01	0.61
1:A:784:LEU:HD12	1:A:785:HIS:N	2.16	0.61
1:A:656:TYR:HA	1:A:684:GLN:O	2.01	0.61
1:C:785:HIS:C	1:C:785:HIS:CD2	2.73	0.60
1:A:693:ILE:HD12	1:A:699:ILE:HD13	1.82	0.60
1:A:603:THR:O	1:A:606:LEU:HD21	2.02	0.60
2:D:108:VAL:O	2:D:115:ILE:HG13	1.95	0.59
1:C:656:TYR:HA	1:C:684:GLN:O	2.03	0.59
2:D:109:LEU:CA	2:D:115:ILE:CD1	2.81	0.59
1:C:616:ILE:CD1	1:C:620:TRP:HB3	2.33	0.58
1:C:693:ILE:HD12	1:C:699:ILE:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:C:309:ARG:NH2	2.37	0.58
2:D:150:ARG:NH1	2:D:153:GLU:OE2	2.36	0.58
1:A:233:ALA:HB2	1:A:243:PHE:HB2	1.84	0.57
2:B:150:ARG:NH1	2:B:153:GLU:OE2	2.38	0.57
2:D:109:LEU:CA	2:D:115:ILE:HG12	2.34	0.56
1:A:340:PHE:CE1	1:A:348:GLY:HA3	2.41	0.56
1:C:484:GLN:HB2	1:C:517:VAL:CG2	2.35	0.56
2:D:156:ILE:HA	2:D:159:LEU:HD12	1.89	0.55
1:C:340:PHE:CE1	1:C:348:GLY:HA3	2.42	0.54
1:A:301:GLU:CD	1:A:301:GLU:H	2.10	0.54
1:C:233:ALA:HB2	1:C:243:PHE:HB2	1.87	0.54
2:D:118:ILE:HG21	2:D:162:ILE:HD11	1.90	0.54
1:C:394:LEU:C	1:C:394:LEU:HD12	2.28	0.54
2:B:118:ILE:HG21	2:B:162:ILE:HD11	1.90	0.53
2:B:156:ILE:HA	2:B:159:LEU:HD12	1.91	0.53
1:C:230:ILE:HD11	1:C:757:GLU:HA	1.90	0.53
1:A:740:ASP:O	1:A:744:GLN:HA	2.09	0.52
1:A:245:LEU:O	1:A:245:LEU:HG	2.10	0.52
1:C:639:ASN:HA	1:C:656:TYR:O	2.10	0.51
1:C:527:ASN:ND2	1:C:530:SER:O	2.36	0.51
1:A:394:LEU:C	1:A:394:LEU:HD12	2.30	0.51
1:C:506:GLN:HG3	1:C:565:ARG:O	2.11	0.51
1:A:292:LEU:O	1:A:309:ARG:HB2	2.09	0.51
1:C:616:ILE:HD13	1:C:620:TRP:CB	2.41	0.51
1:C:302:HIS:N	1:C:303:PRO:CD	2.74	0.51
1:A:297:VAL:C	1:A:301:GLU:OE1	2.45	0.50
1:A:639:ASN:HA	1:A:656:TYR:O	2.10	0.50
1:A:695:ASP:N	1:A:695:ASP:OD1	2.45	0.50
1:C:781:GLN:NE2	2:D:85:ASP:OD2	2.45	0.50
1:C:614:TRP:CZ2	1:C:616:ILE:HG23	2.47	0.50
1:C:395:ASP:OD1	1:C:413:GLN:HG3	2.11	0.50
1:C:740:ASP:O	1:C:744:GLN:HA	2.12	0.50
2:D:110:ILE:N	2:D:115:ILE:HD13	2.26	0.50
1:A:377:PHE:CE2	2:B:134:LEU:HA	2.47	0.50
1:A:694:ALA:O	1:A:696:ARG:N	2.40	0.49
1:A:506:GLN:HG3	1:A:565:ARG:O	2.12	0.49
1:A:324:VAL:HG23	1:A:325:TRP:CD1	2.47	0.49
1:A:369:ASN:OD1	1:A:397:ASN:HB2	2.12	0.49
1:C:279:LEU:HD12	1:C:284:ALA:HB2	1.94	0.49
1:C:454:LEU:HD12	1:C:482:MET:HG3	1.95	0.49
1:A:279:LEU:HD12	1:A:284:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:OD1	1:A:413:GLN:HG3	2.12	0.49
1:C:693:ILE:HD12	1:C:699:ILE:HD11	1.94	0.49
1:A:533:LEU:HD23	2:B:139:GLU:OE2	2.12	0.49
1:A:693:ILE:CD1	1:A:699:ILE:HD13	2.43	0.49
1:C:245:LEU:O	1:C:245:LEU:HD22	2.14	0.48
1:C:693:ILE:CD1	1:C:699:ILE:CD1	2.91	0.48
1:A:527:ASN:ND2	1:A:530:SER:O	2.38	0.48
1:C:694:ALA:C	1:C:696:ARG:H	2.17	0.48
1:A:454:LEU:HD12	1:A:482:MET:HG3	1.96	0.48
1:A:238:THR:HG21	1:A:341:ASN:O	2.14	0.48
1:A:246:PRO:HB3	1:A:260:THR:OG1	2.14	0.48
2:B:86:THR:CG2	2:B:95:THR:HG23	2.35	0.48
1:C:677:GLN:HG2	1:C:678:TYR:CD2	2.49	0.48
1:A:616:ILE:CD1	1:A:620:TRP:HB3	2.44	0.48
1:A:781:GLN:NE2	2:B:85:ASP:OD2	2.46	0.48
2:B:140:GLN:O	2:B:141:ASP:C	2.53	0.47
1:C:230:ILE:HD12	1:C:756:ILE:HB	1.96	0.47
2:D:110:ILE:HB	2:D:113:ARG:HB2	1.96	0.47
1:A:696:ARG:CZ	1:A:696:ARG:HB3	2.44	0.47
1:C:677:GLN:HA	2:D:91:ARG:HB2	1.96	0.47
1:A:233:ALA:HA	1:A:243:PHE:HA	1.97	0.47
1:A:693:ILE:HD12	1:A:699:ILE:CD1	2.45	0.47
1:C:324:VAL:HG23	1:C:325:TRP:CD1	2.49	0.47
1:A:495:ARG:NH1	1:A:499:MET:SD	2.87	0.47
1:C:487:VAL:O	1:C:513:GLN:HA	2.15	0.47
2:D:25:ASP:OD1	2:D:25:ASP:N	2.47	0.46
1:A:299:GLU:O	1:A:303:PRO:HA	2.15	0.46
1:C:623:ARG:NH2	1:C:784:LEU:CD2	2.78	0.46
2:D:140:GLN:O	2:D:141:ASP:C	2.52	0.46
1:C:617:SER:O	1:C:620:TRP:O	2.34	0.46
1:C:694:ALA:O	1:C:696:ARG:N	2.40	0.46
2:D:84:LYS:HE3	2:D:98:TYR:CD2	2.50	0.46
1:A:252:ALA:HB1	1:A:253:PRO:HD2	1.96	0.46
1:A:290:ASP:O	1:A:311:TRP:HA	2.16	0.46
2:B:25:ASP:OD1	2:B:25:ASP:N	2.49	0.46
1:C:380:PHE:O	1:C:381:SER:HB3	2.16	0.46
1:C:369:ASN:OD1	1:C:397:ASN:HB2	2.16	0.46
1:A:241[B]:PHE:CD1	1:A:241[B]:PHE:N	2.80	0.45
1:A:497:MET:O	1:A:501:ALA:O	2.34	0.45
1:C:756:ILE:HG22	1:C:757:GLU:N	2.30	0.45
1:A:756:ILE:HG22	1:A:757:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:C	1:A:324:VAL:H	2.20	0.45
1:C:270:ILE:HG22	1:C:271:MET:O	2.17	0.45
1:C:290:ASP:O	1:C:311:TRP:HA	2.17	0.45
1:A:694:ALA:O	1:A:696:ARG:HG2	2.17	0.45
1:A:312:LEU:HA	1:A:333:LYS:O	2.17	0.45
1:A:693:ILE:O	1:A:697:TRP:HB2	2.17	0.45
1:A:562:VAL:O	1:A:578:SER:HA	2.17	0.45
1:A:581:GLN:HB3	1:A:608:TRP:CE3	2.52	0.45
1:C:246:PRO:HB3	1:C:260:THR:OG1	2.17	0.44
1:C:581:GLN:HB3	1:C:608:TRP:CE3	2.52	0.44
1:A:440:LEU:N	1:A:447:ILE:O	2.49	0.44
1:C:233:ALA:HA	1:C:243:PHE:HA	1.99	0.44
1:C:650:ARG:HD2	1:C:692:PRO:HD3	1.98	0.44
1:A:351:THR:HB	2:B:95:THR:OG1	2.17	0.44
1:A:608:TRP:HB2	1:A:628:TYR:HB3	1.98	0.44
1:A:615:ARG:NH1	1:A:785:HIS:HB2	2.32	0.44
1:A:694:ALA:C	1:A:696:ARG:H	2.19	0.44
1:C:238:THR:HG21	1:C:341:ASN:O	2.17	0.44
1:C:495:ARG:NH1	1:C:499:MET:SD	2.90	0.44
1:A:487:VAL:O	1:A:513:GLN:HA	2.17	0.44
1:C:267:ARG:NH1	1:C:297:VAL:HB	2.32	0.44
2:D:140:GLN:O	2:D:143:ILE:N	2.51	0.44
1:A:244[B]:TYR:CE2	1:A:262:HIS:CD2	3.06	0.44
1:C:497:MET:O	1:C:501:ALA:O	2.36	0.44
1:A:270:ILE:HG22	1:A:271:MET:O	2.18	0.44
1:A:650:ARG:HD2	1:A:692:PRO:HD3	2.00	0.43
1:A:291:TYR:CE1	1:A:309:ARG:HD2	2.54	0.43
2:B:140:GLN:O	2:B:143:ILE:N	2.52	0.43
1:A:495:ARG:HG2	2:B:21:TRP:CH2	2.53	0.43
1:A:232:ASN:HB2	1:A:244[A]:TYR:CD2	2.54	0.43
1:A:676:GLU:HG3	1:A:744:GLN:OE1	2.18	0.43
1:A:677:GLN:HG2	1:A:678:TYR:CD2	2.54	0.43
1:C:608:TRP:HB2	1:C:628:TYR:HB3	2.00	0.43
2:D:159:LEU:N	2:D:160:PRO:CD	2.81	0.43
1:C:562:VAL:O	1:C:578:SER:HA	2.18	0.43
1:C:704:TYR:CG	1:C:778:LEU:HD12	2.54	0.43
1:A:230:ILE:HG13	1:A:230:ILE:O	2.19	0.42
1:A:613:TYR:OH	1:A:615:ARG:HD3	2.19	0.42
1:C:297:VAL:O	1:C:297:VAL:HG12	2.19	0.42
2:D:110:ILE:H	2:D:115:ILE:HD13	1.83	0.42
1:C:440:LEU:N	1:C:447:ILE:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:LEU:HD12	1:C:509:GLU:N	2.34	0.42
1:C:260:THR:HB	1:C:273:GLU:HB2	2.01	0.42
2:D:32:THR:OG1	2:D:163:ARG:NE	2.53	0.42
2:D:86:THR:CG2	2:D:95:THR:HG23	2.36	0.42
1:A:244[B]:TYR:CE2	1:A:262:HIS:CG	3.07	0.42
1:C:784:LEU:CD2	1:C:784:LEU:N	2.82	0.42
1:A:309:ARG:HH11	1:A:309:ARG:HG2	1.84	0.42
1:A:394:LEU:HD12	1:A:395:ASP:N	2.34	0.42
2:B:32:THR:OG1	2:B:163:ARG:NE	2.53	0.42
2:B:128:ASP:OD1	2:B:129:ASN:N	2.53	0.42
1:C:230:ILE:O	1:C:230:ILE:HG13	2.19	0.42
1:C:693:ILE:O	1:C:697:TRP:HB2	2.20	0.41
1:C:288:GLU:OE1	1:C:290:ASP:OD1	2.38	0.41
1:C:613:TYR:OH	1:C:615:ARG:HD3	2.20	0.41
2:B:145:LYS:O	2:B:148:TYR:HB2	2.20	0.41
2:B:84:LYS:HE3	2:B:98:TYR:CD2	2.55	0.41
1:C:355:ALA:N	1:C:380:PHE:HE1	2.18	0.41
2:B:159:LEU:N	2:B:160:PRO:CD	2.84	0.41
1:C:235[B]:TYR:HE1	1:C:241[B]:PHE:HE1	1.53	0.41
1:C:351:THR:HB	2:D:95:THR:OG1	2.20	0.41
1:A:484:GLN:HB2	1:A:517:VAL:CG2	2.46	0.41
2:D:90:PHE:CE2	2:D:96:ALA:HA	2.56	0.41
1:C:252:ALA:HB1	1:C:253:PRO:HD2	2.01	0.41
1:C:394:LEU:HD12	1:C:395:ASP:N	2.36	0.41
1:A:297:VAL:O	1:A:297:VAL:HG12	2.21	0.41
1:A:449:THR:HG22	1:A:487:VAL:HB	2.02	0.41
1:C:609:ALA:HA	1:C:626:ILE:O	2.21	0.41
1:A:709:ALA:HB3	2:B:91:ARG:HD3	2.02	0.41
1:C:488:ASP:HA	1:C:512:ALA:O	2.21	0.41
1:A:288:GLU:OE1	1:A:290:ASP:OD1	2.38	0.41
1:C:618:GLU:O	1:C:619:ARG:HG2	2.21	0.41
2:D:109:LEU:CA	2:D:115:ILE:HD13	2.49	0.41
1:A:340:PHE:CZ	1:A:348:GLY:HA3	2.56	0.40
1:A:634:ASN:OD1	1:A:635:VAL:N	2.54	0.40
1:C:438:LEU:O	1:C:448:ASN:HA	2.21	0.40
2:D:115:ILE:HA	2:D:115:ILE:HD12	1.73	0.40
2:D:128:ASP:OD1	2:D:129:ASN:N	2.55	0.40
1:A:267:ARG:NH1	1:A:297:VAL:HB	2.37	0.40
1:A:482:MET:HA	1:A:483:PRO:HD3	1.92	0.40
1:A:495:ARG:HB3	2:B:21:TRP:CE3	2.56	0.40
1:A:508:LEU:HD12	1:A:509:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ALA:CB	2:B:91:ARG:HD3	2.51	0.40
1:C:232:ASN:HB2	1:C:244[A]:TYR:CD2	2.57	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	560/614 (91%)	504 (90%)	51 (9%)	5 (1%)	17 51
1	C	561/614 (91%)	503 (90%)	51 (9%)	7 (1%)	13 44
2	B	148/175 (85%)	129 (87%)	19 (13%)	0	100 100
2	D	148/175 (85%)	132 (89%)	16 (11%)	0	100 100
All	All	1417/1578 (90%)	1268 (90%)	137 (10%)	12 (1%)	17 53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	PRO
1	A	784	LEU
1	C	695	ASP
1	A	246	PRO
1	C	246	PRO
1	C	483	PRO
1	C	784	LEU
1	A	323	GLN
1	C	323	GLN
1	C	381	SER
1	A	439	PRO
1	C	439	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	496/540 (92%)	444 (90%)	52 (10%)	7 26
1	C	497/540 (92%)	447 (90%)	50 (10%)	7 28
2	B	131/153 (86%)	118 (90%)	13 (10%)	8 29
2	D	131/153 (86%)	117 (89%)	14 (11%)	6 25
All	All	1255/1386 (90%)	1126 (90%)	129 (10%)	7 27

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	THR
1	A	243	PHE
1	A	244[A]	TYR
1	A	244[B]	TYR
1	A	248	TYR
1	A	271	MET
1	A	301	GLU
1	A	302	HIS
1	A	306	ASP
1	A	309	ARG
1	A	312	LEU
1	A	320	VAL
1	A	335	SER
1	A	338	SER
1	A	376	GLN
1	A	394	LEU
1	A	408	THR
1	A	409	ARG
1	A	432	LEU
1	A	438	LEU
1	A	446	SER
1	A	449	THR
1	A	461	THR
1	A	468	SER

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Mol	Chain	Res	Type
1	A	488	ASP
1	A	495	ARG
1	A	496	ASP
1	A	504	TYR
1	A	505	THR
1	A	524	ASP
1	A	532	LEU
1	A	538	SER
1	A	586	THR
1	A	588	SER
1	A	601	ASP
1	A	611	ASP
1	A	612	THR
1	A	616	ILE
1	A	622	LEU
1	A	642	ILE
1	A	676	GLU
1	A	684	GLN
1	A	691	TRP
1	A	695	ASP
1	A	696	ARG
1	A	717	LEU
1	A	719	VAL
1	A	724	CYS
1	A	745	HIS
1	A	774	ARG
1	A	784	LEU
1	A	785	HIS
2	B	25	ASP
2	B	26	THR
2	B	66	GLU
2	B	70	LYS
2	B	76	ARG
2	B	89	VAL
2	B	94	GLN
2	B	95	THR
2	B	101	ILE
2	B	103	THR
2	B	114	ASP
2	B	124	ARG
2	B	161	SER
1	C	238	THR

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Mol	Chain	Res	Type
1	C	243	PHE
1	C	244[A]	TYR
1	C	244[B]	TYR
1	C	245	LEU
1	C	248	TYR
1	C	271	MET
1	C	306	ASP
1	C	309	ARG
1	C	312	LEU
1	C	320	VAL
1	C	322	ASP
1	C	335	SER
1	C	338	SER
1	C	376	GLN
1	C	382	GLU
1	C	394	LEU
1	C	408	THR
1	C	409	ARG
1	C	432	LEU
1	C	438	LEU
1	C	446	SER
1	C	449	THR
1	C	461	THR
1	C	464	ASP
1	C	468	SER
1	C	484	GLN
1	C	488	ASP
1	C	495	ARG
1	C	504	TYR
1	C	505	THR
1	C	524	ASP
1	C	532	LEU
1	C	538	SER
1	C	586	THR
1	C	588	SER
1	C	601	ASP
1	C	612	THR
1	C	616	ILE
1	C	619	ARG
1	C	622	LEU
1	C	642	ILE
1	C	684	GLN

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Mol	Chain	Res	Type
1	C	717	LEU
1	C	719	VAL
1	C	724	CYS
1	C	745	HIS
1	C	774	ARG
1	C	784	LEU
1	C	785	HIS
2	D	25	ASP
2	D	26	THR
2	D	66	GLU
2	D	70	LYS
2	D	76	ARG
2	D	89	VAL
2	D	94	GLN
2	D	95	THR
2	D	101	ILE
2	D	103	THR
2	D	113	ARG
2	D	114	ASP
2	D	124	ARG
2	D	161	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	GLN
1	C	680	ASN
1	C	782	ASN
1	C	785	HIS
2	D	99	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 5 ligands modelled in this entry, 5 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, 95^{th} 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	556/614 (90%)	0.55	45 (8%) 12 13	65, 103, 161, 241	0
1	C	557/614 (90%)	0.50	44 (7%) 12 14	67, 115, 167, 203	0
2	B	150/175 (85%)	0.41	8 (5%) 26 28	71, 118, 177, 199	0
2	D	150/175 (85%)	0.65	16 (10%) 6 7	84, 124, 183, 205	0
All	All	1413/1578 (89%)	0.53	113 (7%) 12 14	65, 112, 171, 241	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	728	ILE	6.6
1	A	762	SER	6.2
1	C	475	ASP	6.2
1	C	760	GLY	6.1
1	C	761	LEU	6.0
2	D	166	ASP	5.7
1	C	763	SER	5.5
1	C	596	THR	5.4
1	A	763	SER	5.1
1	A	727	ALA	5.0
2	D	32	THR	4.9
1	A	756	ILE	4.9
1	A	726	TYR	4.9
1	A	758	LEU	4.5
1	A	598	GLU	4.3
1	C	480	ARG	4.1
1	C	762	SER	4.1
2	B	91	ARG	4.1
1	A	761	LEU	4.0
1	A	467	ASN	4.0
1	C	491	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	466	TYR	3.9
2	D	71	ASP	3.8
2	D	165	ALA	3.8
1	A	757	GLU	3.7
2	D	21	TRP	3.7
1	A	601	ASP	3.6
2	B	71	ASP	3.5
2	B	92	ASN	3.5
1	A	245	LEU	3.5
1	C	477	SER	3.5
1	A	605	SER	3.4
1	A	742	ASP	3.4
1	A	706	ASP	3.3
1	A	754[A]	PHE	3.3
2	B	90	PHE	3.2
2	D	63	LEU	3.2
1	C	281	GLN	3.2
2	B	70	LYS	3.1
1	C	479	ASN	3.1
1	A	729	ARG	3.1
1	C	503	GLY	3.1
1	A	383	GLN	3.0
1	C	298	TYR	3.0
1	A	413	GLN	3.0
2	D	33	MET	3.0
1	C	465	TRP	3.0
1	C	759	ARG	2.9
1	C	598	GLU	2.9
2	D	163	ARG	2.9
1	C	299	GLU	2.9
1	A	760	GLY	2.9
1	A	395	ASP	2.9
1	A	765	TYR	2.9
1	C	464	ASP	2.9
2	D	31	SER	2.9
1	C	493	PHE	2.9
1	A	508	LEU	2.8
1	C	431	HIS	2.8
1	A	596	THR	2.8
2	B	109	LEU	2.8
1	A	678	TYR	2.8
1	C	486	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	764	ASN	2.8
1	A	747	VAL	2.8
2	B	38	LEU	2.8
1	A	739	TRP	2.7
1	C	457	HIS	2.7
1	A	537	TYR	2.6
1	C	325	TRP	2.6
1	C	485	PHE	2.6
1	C	752	ILE	2.6
1	C	521	ASP	2.6
1	C	508	LEU	2.6
1	C	458	TYR	2.5
1	A	602	LYS	2.5
2	D	104	VAL	2.5
1	C	460	GLN	2.5
1	C	510	PRO	2.5
2	D	92	ASN	2.5
1	C	469	ARG	2.5
1	A	606	LEU	2.4
1	C	741	ASN	2.4
1	A	759	ARG	2.4
1	A	497	MET	2.4
1	C	254	ASN	2.4
1	A	298	TYR	2.4
1	C	463	LEU	2.4
2	B	20	GLY	2.3
1	A	483	PRO	2.3
1	A	244[A]	TYR	2.3
1	A	472	THR	2.3
1	C	383	GLN	2.3
1	C	413	GLN	2.3
2	D	75	LEU	2.3
1	A	591	GLY	2.3
1	A	755	ASN	2.3
1	C	611	ASP	2.3
1	A	724	CYS	2.3
1	C	667	THR	2.3
1	A	415	VAL	2.3
1	A	518	PRO	2.2
1	C	562	VAL	2.2
1	A	676	GLU	2.2
2	D	37	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	599	ASN	2.2
1	C	672	TYR	2.1
1	C	662	GLU	2.1
2	D	167	ILE	2.1
1	A	736	LEU	2.0
2	D	69	ARG	2.0
2	D	97	GLU	2.0
1	A	516	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, 95^{th} 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	CL	A	801	1/1	0.52	0.28	104,104,104,104	0
3	CL	C	803	1/1	0.57	0.34	102,102,102,102	0
4	NA	B	201	1/1	0.80	0.55	65,65,65,65	0
3	CL	C	802	1/1	0.90	0.30	83,83,83,83	0
3	CL	C	801	1/1	0.94	0.36	89,89,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.