



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:32 AM UTC

PDB ID : 1OSM / pdb_00001osm
Title : OSMOPORIN (OMPK36) FROM KLEBSIELLA PNEUMONIAE
Authors : Dutzler, R.; Schirmer, T.
Deposited on : 1999-01-08
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

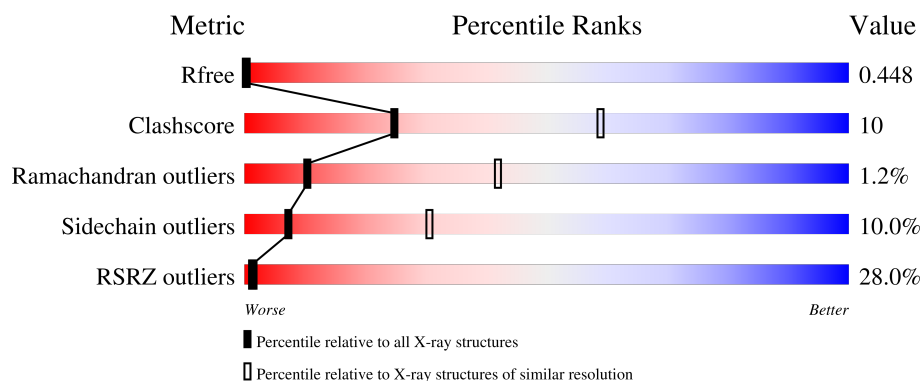
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	342	29% 77% 19% 5%
1	B	342	26% 78% 17% 5%
1	C	342	29% 78% 18% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D12	A	342	-	-	X	-
2	D12	A	345	-	-	X	-
2	D12	A	348	-	-	X	-
2	D12	A	349	-	-	X	-

2 Entry composition [i](#)

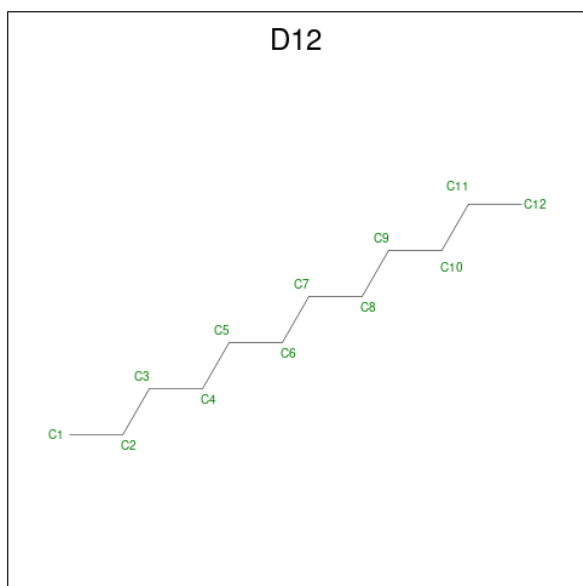
There are 2 unique types of molecules in this entry. The entry contains 8100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMPK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			
1	B	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			
1	C	342	Total	C	N	O	S	0	0	0
			2664	1670	442	550	2			

- Molecule 2 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			12	12		
2	A	1	Total	C	0	0
			12	12		
2	A	1	Total	C	0	0
			12	12		

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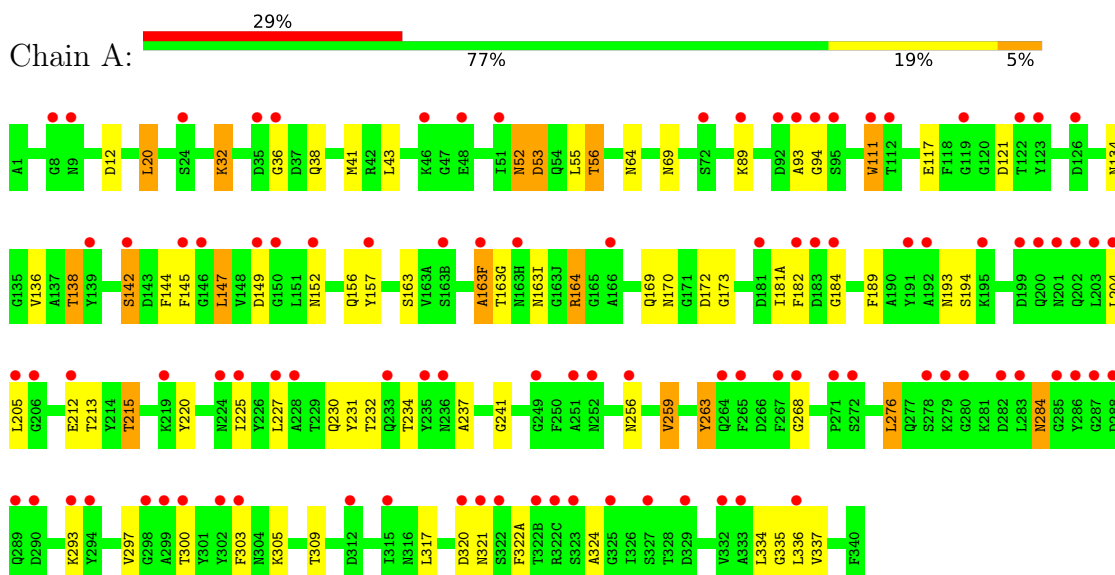
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0

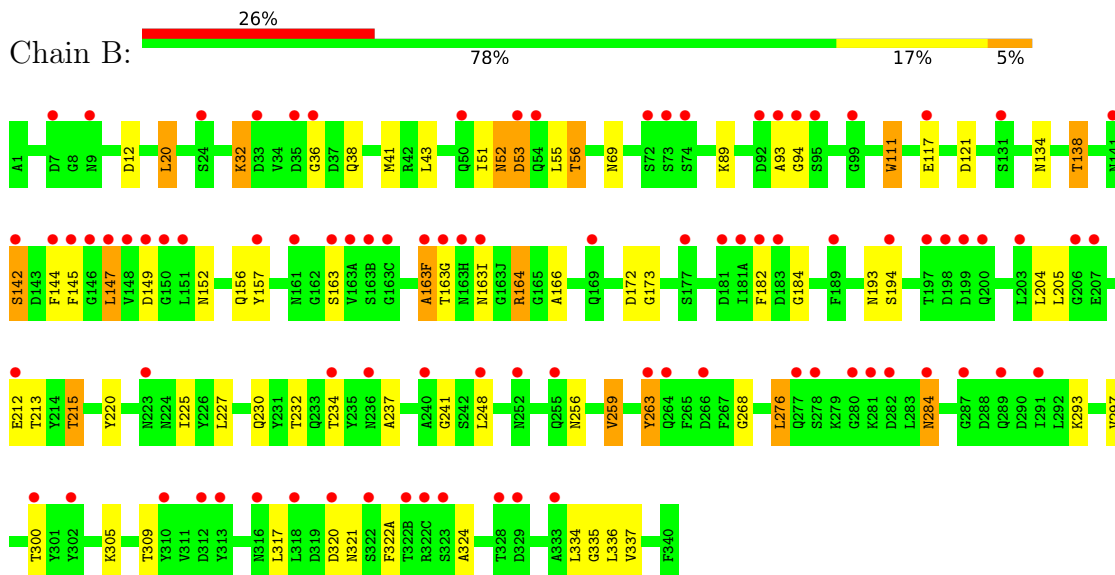
3 Residue-property plots [i](#)

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.

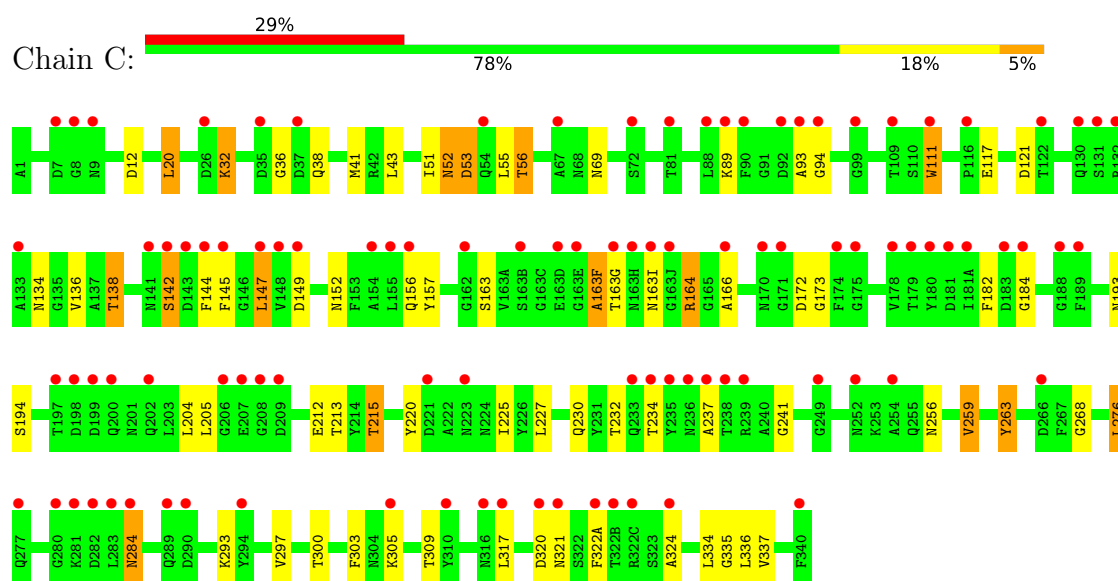
• Molecule 1: OMPK36



• Molecule 1: OMPK36



• Molecule 1: OMPK36



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.80Å 76.80Å 223.40Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (15.00-3.20) 95.1 (15.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.19Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.208 , 0.223 0.443 , 0.448	Depositor DCC
R_{free} test set	4740 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	8100	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D12

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	0.75	0/2720	1.07	14/3682 (0.4%)
1	B	0.75	0/2720	1.07	14/3682 (0.4%)
1	C	0.75	0/2720	1.07	15/3682 (0.4%)
All	All	0.75	0/8160	1.07	43/11046 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	GLY	N-CA-C	7.25	122.27	113.79
1	C	268	GLY	N-CA-C	7.23	122.25	113.79
1	A	268	GLY	N-CA-C	7.23	122.25	113.79
1	A	142	SER	N-CA-C	7.21	126.16	110.80
1	B	142	SER	N-CA-C	7.20	126.14	110.80
1	C	142	SER	N-CA-C	7.19	126.11	110.80
1	C	94	GLY	N-CA-C	6.92	118.41	111.21
1	C	121	ASP	N-CA-C	6.92	121.63	111.87
1	A	121	ASP	N-CA-C	6.92	121.62	111.87
1	A	94	GLY	N-CA-C	6.90	118.39	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	N-CA-C	6.90	121.59	111.87
1	C	36	GLY	N-CA-C	6.86	121.56	111.76
1	A	36	GLY	N-CA-C	6.80	121.49	111.76
1	B	36	GLY	N-CA-C	6.80	121.49	111.76
1	B	94	GLY	N-CA-C	6.80	118.28	111.21
1	B	53	ASP	N-CA-C	-6.60	105.04	113.23
1	C	53	ASP	N-CA-C	-6.59	105.06	113.23
1	A	53	ASP	N-CA-C	-6.56	105.10	113.23
1	C	337	VAL	N-CA-C	5.67	116.84	108.45
1	B	337	VAL	N-CA-C	5.65	116.81	108.45
1	A	337	VAL	N-CA-C	5.65	116.81	108.45
1	B	138	THR	N-CA-C	5.45	117.97	108.76
1	C	163(G)	THR	N-CA-C	-5.45	100.79	109.07
1	A	163(G)	THR	N-CA-C	-5.41	100.84	109.07
1	B	163(G)	THR	N-CA-C	-5.41	100.84	109.07
1	A	138	THR	N-CA-C	5.41	117.90	108.76
1	B	111	TRP	CA-CB-CG	5.40	123.86	113.60
1	A	111	TRP	CA-CB-CG	5.39	123.84	113.60
1	C	111	TRP	CA-CB-CG	5.38	123.83	113.60
1	C	138	THR	N-CA-C	5.36	117.81	108.76
1	B	259	VAL	CB-CA-C	-5.33	101.85	110.28
1	A	259	VAL	CB-CA-C	-5.32	101.88	110.28
1	C	259	VAL	CB-CA-C	-5.31	101.90	110.28
1	C	335	GLY	N-CA-C	5.30	120.94	111.03
1	A	335	GLY	N-CA-C	5.30	120.93	111.03
1	B	335	GLY	N-CA-C	5.28	120.90	111.03
1	B	52	ASN	CB-CA-C	-5.27	101.26	114.11
1	A	52	ASN	CB-CA-C	-5.26	101.27	114.11
1	C	52	ASN	CB-CA-C	-5.25	101.30	114.11
1	C	136	VAL	N-CA-C	5.06	115.14	107.80
1	B	166	ALA	N-CA-C	5.03	119.68	111.37
1	A	136	VAL	N-CA-C	5.03	115.09	107.80
1	C	166	ALA	N-CA-C	5.01	119.64	111.37

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	TYR	Sidechain
1	B	263	TYR	Sidechain
1	C	263	TYR	Sidechain

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	2664	0	2452	45	0
1	B	2664	0	2452	43	0
1	C	2664	0	2452	43	0
2	A	108	0	234	33	0
All	All	8100	0	7590	154	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 (154) 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:A:189:PHE:HB3	2:A:349:D12:H13	1.45	0.98
2:A:345:D12:H102	2:A:348:D12:H112	1.48	0.96
2:A:348:D12:H62	2:A:349:D12:H41	1.55	0.88
2:A:345:D12:H123	2:A:348:D12:C11	2.04	0.86
2:A:348:D12:H71	2:A:349:D12:H61	1.60	0.83
1:B:173:GLY:HA3	1:B:194:SER:HB3	1.60	0.83
1:C:173:GLY:HA3	1:C:194:SER:HB3	1.60	0.83
1:A:173:GLY:HA3	1:A:194:SER:HB3	1.60	0.82
1:B:215:THR:HB	1:B:232:THR:OG1	1.83	0.79
1:A:215:THR:HB	1:A:232:THR:OG1	1.83	0.78
1:C:215:THR:HB	1:C:232:THR:OG1	1.83	0.78
2:A:345:D12:H102	2:A:348:D12:C11	2.16	0.76
1:A:163(I):ASN:O	1:A:164:ARG:NH1	2.20	0.74
1:B:163(I):ASN:O	1:B:164:ARG:NH1	2.20	0.74
1:C:163(I):ASN:O	1:C:164:ARG:NH1	2.21	0.74
2:A:342:D12:H42	2:A:349:D12:H112	1.73	0.69
2:A:345:D12:H123	2:A:348:D12:H111	1.74	0.68
1:A:181(A):ILE:HD13	2:A:348:D12:H123	1.76	0.68
1:C:163(I):ASN:HD22	1:C:163(I):ASN:H	1.43	0.67
1:A:147:LEU:HD12	1:A:147:LEU:N	2.10	0.66
1:A:163(F):ALA:O	1:B:32:LYS:HD2	1.95	0.66
1:C:147:LEU:N	1:C:147:LEU:HD12	2.10	0.66
1:B:147:LEU:HD12	1:B:147:LEU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PHE:HB2	1:B:147:LEU:HD13	1.78	0.66
1:A:145:PHE:HB2	1:A:147:LEU:HD13	1.78	0.65
1:C:145:PHE:HB2	1:C:147:LEU:HD13	1.78	0.65
1:A:163(I):ASN:H	1:A:163(I):ASN:HD22	1.43	0.64
1:B:157:TYR:OH	1:B:172:ASP:HB3	1.98	0.64
1:C:134:ASN:ND2	1:C:164:ARG:NH2	2.46	0.64
1:A:157:TYR:OH	1:A:172:ASP:HB3	1.98	0.64
1:B:134:ASN:ND2	1:B:164:ARG:NH2	2.46	0.63
1:B:163(I):ASN:HD22	1:B:163(I):ASN:H	1.43	0.63
2:A:345:D12:H123	2:A:348:D12:C12	2.28	0.63
1:C:157:TYR:OH	1:C:172:ASP:HB3	1.98	0.63
2:A:345:D12:H123	2:A:348:D12:H121	1.80	0.63
1:A:134:ASN:ND2	1:A:164:ARG:NH2	2.46	0.62
2:A:342:D12:C12	2:A:347:D12:H112	2.30	0.62
2:A:345:D12:C10	2:A:348:D12:H112	2.28	0.61
1:B:163(F):ALA:O	1:C:32:LYS:HD2	2.01	0.61
1:B:321:ASN:ND2	1:B:322(A):PHE:H	2.00	0.60
2:A:345:D12:H82	2:A:348:D12:H92	1.84	0.59
2:A:346:D12:H112	2:A:349:D12:H21	1.85	0.59
1:C:321:ASN:ND2	1:C:322(A):PHE:H	2.00	0.58
1:A:321:ASN:ND2	1:A:322(A):PHE:H	2.00	0.58
1:B:293:LYS:HG2	1:B:317:LEU:HB2	1.86	0.58
2:A:345:D12:H62	2:A:348:D12:H52	1.86	0.58
1:A:32:LYS:HD2	1:C:163(F):ALA:O	2.04	0.58
1:C:284:ASN:HD22	1:C:284:ASN:N	2.02	0.57
1:C:293:LYS:HG2	1:C:317:LEU:HB2	1.86	0.57
1:A:293:LYS:HG2	1:A:317:LEU:HB2	1.86	0.57
2:A:345:D12:H82	2:A:348:D12:H72	1.87	0.57
1:A:41:MET:HE1	1:A:43:LEU:HB2	1.87	0.57
1:A:241:GLY:HA3	1:A:324:ALA:HB1	1.87	0.57
1:B:284:ASN:HD22	1:B:284:ASN:N	2.02	0.57
1:A:284:ASN:HD22	1:A:284:ASN:N	2.02	0.56
1:C:41:MET:HE1	1:C:43:LEU:HB2	1.87	0.56
1:C:241:GLY:HA3	1:C:324:ALA:HB1	1.87	0.56
1:C:134:ASN:HD22	1:C:164:ARG:NH2	2.04	0.56
1:B:241:GLY:HA3	1:B:324:ALA:HB1	1.87	0.56
1:A:134:ASN:HD22	1:A:164:ARG:HH21	1.53	0.55
1:B:41:MET:HE1	1:B:43:LEU:HB2	1.87	0.55
1:B:134:ASN:HD22	1:B:164:ARG:NH2	2.04	0.55
1:B:134:ASN:HD22	1:B:164:ARG:HH21	1.53	0.55
1:B:215:THR:HB	1:B:232:THR:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:HD22	1:A:164:ARG:NH2	2.04	0.54
1:C:134:ASN:HD22	1:C:164:ARG:HH21	1.53	0.54
1:C:215:THR:HB	1:C:232:THR:CB	2.37	0.54
2:A:345:D12:H62	2:A:348:D12:C5	2.37	0.54
1:B:20:LEU:HB3	1:B:38:GLN:HB2	1.88	0.54
2:A:342:D12:H122	2:A:347:D12:H112	1.90	0.54
1:A:215:THR:HB	1:A:232:THR:CB	2.37	0.53
1:C:20:LEU:HB3	1:C:38:GLN:HB2	1.89	0.53
1:A:20:LEU:HB3	1:A:38:GLN:HB2	1.89	0.53
2:A:342:D12:H123	2:A:347:D12:H112	1.92	0.52
1:B:147:LEU:N	1:B:147:LEU:CD1	2.73	0.52
1:C:147:LEU:N	1:C:147:LEU:CD1	2.73	0.52
2:A:348:D12:H62	2:A:349:D12:C4	2.34	0.51
2:A:345:D12:H112	2:A:347:D12:H111	1.92	0.51
1:A:147:LEU:N	1:A:147:LEU:CD1	2.73	0.50
1:C:52:ASN:HB2	1:C:55:LEU:H	1.77	0.50
1:B:51:ILE:HD13	1:C:303:PHE:HB3	1.94	0.50
1:A:303:PHE:HB3	1:C:51:ILE:HD13	1.92	0.49
1:A:52:ASN:HB2	1:A:55:LEU:H	1.77	0.49
1:B:225:ILE:HD13	1:B:263:TYR:HD1	1.78	0.49
1:C:225:ILE:HD13	1:C:263:TYR:HD1	1.78	0.49
2:A:341:D12:H82	2:A:342:D12:H72	1.94	0.49
2:A:345:D12:H62	2:A:348:D12:H72	1.95	0.49
1:C:157:TYR:OH	1:C:172:ASP:CB	2.61	0.49
1:A:157:TYR:OH	1:A:172:ASP:CG	2.56	0.49
1:B:52:ASN:HB2	1:B:55:LEU:H	1.77	0.49
1:C:157:TYR:OH	1:C:172:ASP:CG	2.56	0.49
1:B:157:TYR:OH	1:B:172:ASP:CB	2.61	0.48
1:B:157:TYR:OH	1:B:172:ASP:CG	2.56	0.48
1:B:184:GLY:O	1:B:220:TYR:HA	2.14	0.48
1:C:184:GLY:O	1:C:220:TYR:HA	2.14	0.48
1:A:184:GLY:O	1:A:220:TYR:HA	2.14	0.48
1:A:225:ILE:HD13	1:A:263:TYR:HD1	1.78	0.47
2:A:345:D12:H102	2:A:348:D12:H92	1.95	0.47
1:A:157:TYR:OH	1:A:172:ASP:CB	2.61	0.47
2:A:345:D12:H112	2:A:347:D12:C12	2.44	0.47
2:A:342:D12:C4	2:A:349:D12:H112	2.43	0.47
2:A:346:D12:C11	2:A:349:D12:H21	2.44	0.46
1:A:52:ASN:HB3	1:A:53:ASP:H	1.54	0.46
1:A:147:LEU:HD12	1:A:147:LEU:H	1.81	0.46
1:C:147:LEU:CD1	1:C:147:LEU:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD12	1:B:147:LEU:H	1.81	0.46
1:A:189:PHE:HB2	2:A:349:D12:H31	1.98	0.46
1:A:276:LEU:HD23	1:A:276:LEU:N	2.31	0.46
1:A:147:LEU:CD1	1:A:147:LEU:H	2.28	0.46
1:B:276:LEU:N	1:B:276:LEU:HD23	2.31	0.46
1:B:234:THR:HB	1:B:237:ALA:HB3	1.99	0.45
1:C:234:THR:HB	1:C:237:ALA:HB3	1.98	0.45
2:A:345:D12:C12	2:A:348:D12:C11	2.88	0.45
1:B:147:LEU:CD1	1:B:147:LEU:H	2.28	0.45
1:A:234:THR:HB	1:A:237:ALA:HB3	1.98	0.45
1:B:52:ASN:HB3	1:B:53:ASP:H	1.54	0.45
1:C:276:LEU:N	1:C:276:LEU:HD23	2.31	0.45
1:C:147:LEU:HD12	1:C:147:LEU:H	1.81	0.45
1:B:193:ASN:HD22	1:B:212:GLU:HG2	1.82	0.45
1:A:56:THR:HG23	1:A:89:LYS:HB3	1.99	0.45
1:C:56:THR:HG23	1:C:89:LYS:HB3	1.99	0.45
1:A:163:SER:O	1:A:163(F):ALA:HA	2.18	0.44
2:A:342:D12:H62	2:A:349:D12:H112	1.99	0.44
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.78	0.44
1:B:56:THR:HG23	1:B:89:LYS:HB3	1.99	0.44
1:C:193:ASN:HD22	1:C:212:GLU:HG2	1.82	0.44
1:A:204:LEU:HG	1:A:205:LEU:HD12	1.99	0.44
1:B:204:LEU:HG	1:B:205:LEU:HD12	2.00	0.44
1:B:144:PHE:O	1:B:145:PHE:HB2	2.18	0.44
1:C:163:SER:O	1:C:163(F):ALA:HA	2.18	0.44
1:C:204:LEU:HG	1:C:205:LEU:HD12	2.00	0.44
2:A:342:D12:H62	2:A:349:D12:C11	2.48	0.43
1:C:32:LYS:HD3	1:C:32:LYS:HA	1.65	0.43
1:A:193:ASN:HD22	1:A:212:GLU:HG2	1.82	0.43
1:B:163:SER:O	1:B:163(F):ALA:HA	2.18	0.43
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.65	0.43
1:C:205:LEU:HD12	1:C:205:LEU:N	2.34	0.43
1:A:205:LEU:HD12	1:A:205:LEU:N	2.34	0.43
1:C:134:ASN:ND2	1:C:164:ARG:HH21	2.13	0.43
1:B:134:ASN:ND2	1:B:164:ARG:HH21	2.13	0.43
1:C:52:ASN:HB3	1:C:53:ASP:H	1.54	0.43
1:B:205:LEU:HD12	1:B:205:LEU:N	2.34	0.42
1:C:144:PHE:O	1:C:145:PHE:HB2	2.18	0.42
1:A:231:TYR:HB3	2:A:349:D12:H111	2.01	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.77	0.42
1:A:144:PHE:O	1:A:145:PHE:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163(F):ALA:O	1:C:32:LYS:HG3	2.19	0.42
1:A:134:ASN:ND2	1:A:164:ARG:HH21	2.13	0.41
1:B:232:THR:HG22	1:B:256:ASN:HB2	2.03	0.41
1:A:169:GLN:O	1:A:170:ASN:HB3	2.21	0.41
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.91	0.40
1:A:232:THR:HG22	1:A:256:ASN:HB2	2.03	0.40
1:B:205:LEU:HD13	1:B:248:LEU:HB3	2.03	0.40
1:C:232:THR:HG22	1:C:256:ASN:HB2	2.03	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	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	10	42
1	B	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	10	42
1	C	340/342 (99%)	313 (92%)	23 (7%)	4 (1%)	10	42
All	All	1020/1026 (99%)	939 (92%)	69 (7%)	12 (1%)	10	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163(F)	ALA
1	B	163(F)	ALA
1	C	163(F)	ALA
1	A	147	LEU
1	B	147	LEU
1	C	147	LEU
1	A	93	ALA
1	B	93	ALA
1	C	93	ALA

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Mol	Chain	Res	Type
1	A	182	PHE
1	B	182	PHE
1	C	182	PHE

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	272/272 (100%)	244 (90%)	28 (10%)	7	28
1	B	272/272 (100%)	245 (90%)	27 (10%)	7	31
1	C	272/272 (100%)	245 (90%)	27 (10%)	7	31
All	All	816/816 (100%)	734 (90%)	82 (10%)	7	30

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	20	LEU
1	A	32	LYS
1	A	56	THR
1	A	64	ASN
1	A	69	ASN
1	A	111	TRP
1	A	117	GLU
1	A	138	THR
1	A	142	SER
1	A	149	ASP
1	A	152	ASN
1	A	156	GLN
1	A	164	ARG
1	A	213	THR
1	A	215	THR
1	A	227	LEU
1	A	230	GLN
1	A	259	VAL

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	284	ASN
1	A	297	VAL
1	A	300	THR
1	A	305	LYS
1	A	309	THR
1	A	320	ASP
1	A	334	LEU
1	A	336	LEU
1	B	12	ASP
1	B	20	LEU
1	B	32	LYS
1	B	56	THR
1	B	69	ASN
1	B	111	TRP
1	B	117	GLU
1	B	138	THR
1	B	142	SER
1	B	149	ASP
1	B	152	ASN
1	B	156	GLN
1	B	164	ARG
1	B	213	THR
1	B	215	THR
1	B	227	LEU
1	B	230	GLN
1	B	259	VAL
1	B	276	LEU
1	B	284	ASN
1	B	297	VAL
1	B	300	THR
1	B	305	LYS
1	B	309	THR
1	B	320	ASP
1	B	334	LEU
1	B	336	LEU
1	C	12	ASP
1	C	20	LEU
1	C	32	LYS
1	C	56	THR
1	C	69	ASN
1	C	111	TRP

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Mol	Chain	Res	Type
1	C	117	GLU
1	C	138	THR
1	C	142	SER
1	C	149	ASP
1	C	152	ASN
1	C	156	GLN
1	C	164	ARG
1	C	213	THR
1	C	215	THR
1	C	227	LEU
1	C	230	GLN
1	C	259	VAL
1	C	276	LEU
1	C	284	ASN
1	C	297	VAL
1	C	300	THR
1	C	305	LYS
1	C	309	THR
1	C	320	ASP
1	C	334	LEU
1	C	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	134	ASN
1	A	163(I)	ASN
1	A	193	ASN
1	A	202	GLN
1	A	252	ASN
1	A	284	ASN
1	A	289	GLN
1	A	316	ASN
1	A	321	ASN
1	B	60	GLN
1	B	134	ASN
1	B	163(I)	ASN
1	B	193	ASN
1	B	201	ASN
1	B	202	GLN
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	284	ASN
1	B	289	GLN
1	B	306	ASN
1	B	316	ASN
1	B	321	ASN
1	C	60	GLN
1	C	134	ASN
1	C	163(I)	ASN
1	C	193	ASN
1	C	202	GLN
1	C	252	ASN
1	C	284	ASN
1	C	289	GLN
1	C	316	ASN
1	C	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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
2	D12	A	346	-	11,11,11	0.39	0	10,10,10	0.63	0
2	D12	A	344	-	11,11,11	0.48	0	10,10,10	0.58	0
2	D12	A	349	-	11,11,11	0.30	0	10,10,10	0.74	0
2	D12	A	347	-	11,11,11	0.45	0	10,10,10	0.55	0
2	D12	A	348	-	11,11,11	0.29	0	10,10,10	0.71	0
2	D12	A	345	-	11,11,11	0.37	0	10,10,10	0.63	0
2	D12	A	341	-	11,11,11	0.33	0	10,10,10	0.66	0
2	D12	A	342	-	11,11,11	0.41	0	10,10,10	0.61	0
2	D12	A	343	-	11,11,11	0.34	0	10,10,10	0.67	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
2	D12	A	346	-	-	1/9/9/9	-
2	D12	A	344	-	-	2/9/9/9	-
2	D12	A	349	-	-	0/9/9/9	-
2	D12	A	347	-	-	0/9/9/9	-
2	D12	A	348	-	-	1/9/9/9	-
2	D12	A	345	-	-	0/9/9/9	-
2	D12	A	341	-	-	1/9/9/9	-
2	D12	A	342	-	-	0/9/9/9	-
2	D12	A	343	-	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	341	D12	C6-C7-C8-C9
2	A	344	D12	C5-C6-C7-C8
2	A	348	D12	C7-C8-C9-C10
2	A	346	D12	C5-C6-C7-C8
2	A	344	D12	C2-C3-C4-C5
2	A	343	D12	C4-C5-C6-C7
2	A	343	D12	C7-C8-C9-C10

There are no ring outliers.

7 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	346	D12	2	0
2	A	349	D12	12	0
2	A	347	D12	5	0
2	A	348	D12	18	0
2	A	345	D12	16	0
2	A	341	D12	1	0
2	A	342	D12	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/342 (100%)	1.56	98 (28%)  	28, 51, 78, 97	0
1	B	342/342 (100%)	1.59	89 (26%)  	28, 51, 78, 97	0
1	C	342/342 (100%)	1.55	100 (29%)  	28, 51, 78, 97	0
All	All	1026/1026 (100%)	1.57	287 (27%)  	28, 51, 78, 97	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	PHE	8.0
1	A	322(B)	THR	6.3
1	B	92	ASP	5.7
1	B	163(A)	VAL	5.6
1	C	163(E)	GLY	5.4
1	B	287	GLY	5.3
1	C	181(A)	ILE	5.1
1	A	322(C)	ARG	5.1
1	B	149	ASP	5.1
1	C	322(A)	PHE	4.7
1	B	150	GLY	4.7
1	B	181(A)	ILE	4.7
1	A	201	ASN	4.6
1	B	206	GLY	4.6
1	B	280	GLY	4.6
1	A	252	ASN	4.6
1	C	163(I)	ASN	4.5
1	C	252	ASN	4.5
1	B	148	VAL	4.5
1	A	299	ALA	4.4
1	A	283	LEU	4.3
1	B	316	ASN	4.3
1	C	9	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	9	ASN	4.2
1	C	93	ALA	4.2
1	B	328	THR	4.1
1	B	145	PHE	4.1
1	C	54	GLN	4.0
1	C	181	ASP	4.0
1	A	298	GLY	3.9
1	C	149	ASP	3.9
1	A	94	GLY	3.9
1	A	51	ILE	3.9
1	B	33	ASP	3.9
1	A	336	LEU	3.9
1	C	184	GLY	3.8
1	C	147	LEU	3.8
1	C	144	PHE	3.7
1	A	9	ASN	3.7
1	A	182	PHE	3.7
1	C	208	GLY	3.7
1	C	178	VAL	3.7
1	B	323	SER	3.6
1	C	156	GLN	3.6
1	A	279	LYS	3.6
1	A	36	GLY	3.6
1	C	207	GLU	3.6
1	C	254	ALA	3.6
1	A	205	LEU	3.6
1	B	163(G)	THR	3.6
1	B	322(B)	THR	3.5
1	B	50	GLN	3.5
1	A	150	GLY	3.5
1	A	157	TYR	3.5
1	A	203	LEU	3.5
1	A	142	SER	3.5
1	A	93	ALA	3.4
1	C	143	ASP	3.4
1	C	290	ASP	3.4
1	A	200	GLN	3.4
1	A	329	ASP	3.4
1	C	198	ASP	3.4
1	C	163(G)	THR	3.4
1	B	322(C)	ARG	3.3
1	C	281	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	3.3
1	B	54	GLN	3.3
1	C	130	GLN	3.3
1	C	321	ASN	3.3
1	B	203	LEU	3.2
1	A	224	ASN	3.2
1	C	283	LEU	3.2
1	B	181	ASP	3.2
1	C	26	ASP	3.2
1	B	281	LYS	3.2
1	B	223	ASN	3.2
1	A	315	ILE	3.2
1	B	35	ASP	3.1
1	B	146	GLY	3.1
1	C	170	ASN	3.1
1	B	329	ASP	3.1
1	B	212	GLU	3.1
1	B	236	ASN	3.1
1	B	252	ASN	3.1
1	C	109	THR	3.1
1	C	294	TYR	3.1
1	B	74	SER	3.1
1	C	142	SER	3.1
1	A	265	PHE	3.1
1	B	197	THR	3.0
1	C	72	SER	3.0
1	C	289	GLN	3.0
1	C	132	ARG	3.0
1	B	291	ILE	3.0
1	B	300	THR	3.0
1	A	219	LYS	3.0
1	A	320	ASP	3.0
1	C	317	LEU	2.9
1	B	310	TYR	2.9
1	A	35	ASP	2.9
1	C	7	ASP	2.9
1	A	282	ASP	2.9
1	A	8	GLY	2.9
1	C	162	GLY	2.9
1	C	180	TYR	2.9
1	C	322(C)	ARG	2.9
1	B	147	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	2.9
1	B	198	ASP	2.8
1	C	141	ASN	2.8
1	A	195	LYS	2.8
1	C	90	PHE	2.8
1	A	288	ASP	2.8
1	A	280	GLY	2.8
1	A	286	TYR	2.8
1	C	235	TYR	2.8
1	B	163(H)	ASN	2.8
1	A	323	SER	2.8
1	C	322(B)	THR	2.8
1	B	199	ASP	2.7
1	A	72	SER	2.7
1	A	290	ASP	2.7
1	B	7	ASP	2.7
1	A	300	THR	2.7
1	B	194	SER	2.7
1	A	92	ASP	2.7
1	B	313	TYR	2.7
1	A	256	ASN	2.7
1	B	302	TYR	2.7
1	C	209	ASP	2.7
1	C	148	VAL	2.7
1	A	267	PHE	2.7
1	B	93	ALA	2.7
1	A	149	ASP	2.7
1	A	202	GLN	2.6
1	A	264	GLN	2.6
1	B	289	GLN	2.6
1	A	119	GLY	2.6
1	A	327	SER	2.6
1	B	163	SER	2.6
1	A	123	TYR	2.6
1	A	228	ALA	2.6
1	B	312	ASP	2.6
1	C	37	ASP	2.6
1	C	280	GLY	2.6
1	C	320	ASP	2.6
1	B	284	ASN	2.6
1	B	207	GLU	2.6
1	A	146	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	199	ASP	2.6
1	C	122	THR	2.6
1	B	163(B)	SER	2.5
1	B	36	GLY	2.5
1	B	163(I)	ASN	2.5
1	B	73	SER	2.5
1	C	233	GLN	2.5
1	A	166	ALA	2.5
1	C	189	PHE	2.5
1	B	163(F)	ALA	2.5
1	C	316	ASN	2.5
1	A	287	GLY	2.5
1	B	94	GLY	2.5
1	C	202	GLN	2.5
1	A	212	GLU	2.5
1	A	236	ASN	2.5
1	C	179	THR	2.5
1	B	99	GLY	2.5
1	B	200	GLN	2.5
1	B	131	SER	2.4
1	C	163(B)	SER	2.4
1	B	117	GLU	2.4
1	B	266	ASP	2.4
1	C	236	ASN	2.4
1	A	285	GLY	2.4
1	A	204	LEU	2.4
1	C	284	ASN	2.4
1	A	312	ASP	2.4
1	C	35	ASP	2.4
1	A	191	TYR	2.4
1	C	175	GLY	2.4
1	C	305	LYS	2.4
1	C	163(H)	ASN	2.4
1	A	249	GLY	2.4
1	A	325	GLY	2.4
1	C	133	ALA	2.4
1	C	145	PHE	2.4
1	B	157	TYR	2.4
1	A	112	THR	2.3
1	B	163(C)	GLY	2.3
1	A	152	ASN	2.3
1	A	289	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	322	SER	2.3
1	C	234	THR	2.3
1	A	199	ASP	2.3
1	B	255	GLN	2.3
1	A	48	GLU	2.3
1	C	163(J)	GLY	2.3
1	B	333	ALA	2.3
1	A	302	TYR	2.3
1	A	126	ASP	2.3
1	B	282	ASP	2.3
1	C	277	GLN	2.3
1	A	225	ILE	2.3
1	A	272	SER	2.3
1	B	144	PHE	2.3
1	C	340	PHE	2.3
1	C	92	ASP	2.3
1	C	282	ASP	2.3
1	A	89	LYS	2.3
1	C	239	ARG	2.3
1	A	206	GLY	2.3
1	C	8	GLY	2.3
1	C	99	GLY	2.3
1	B	234	THR	2.3
1	B	318	LEU	2.3
1	B	95	SER	2.3
1	B	240	ALA	2.2
1	A	111	TRP	2.2
1	B	177	SER	2.2
1	A	321	ASN	2.2
1	B	264	GLN	2.2
1	C	183	ASP	2.2
1	B	248	LEU	2.2
1	C	155	LEU	2.2
1	C	111	TRP	2.2
1	A	145	PHE	2.2
1	C	310	TYR	2.2
1	B	320	ASP	2.2
1	C	206	GLY	2.2
1	A	332	VAL	2.2
1	B	278	SER	2.2
1	C	131	SER	2.2
1	B	277	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	141	ASN	2.2
1	A	271	PRO	2.2
1	C	67	ALA	2.2
1	C	324	ALA	2.2
1	C	266	ASP	2.2
1	B	189	PHE	2.2
1	C	81	THR	2.2
1	C	197	THR	2.2
1	A	95	SER	2.2
1	B	142	SER	2.2
1	B	151	LEU	2.2
1	C	223	ASN	2.2
1	A	181	ASP	2.2
1	B	24	SER	2.1
1	B	72	SER	2.1
1	C	154	ALA	2.1
1	C	94	GLY	2.1
1	C	116	PRO	2.1
1	A	139	TYR	2.1
1	B	263	TYR	2.1
1	A	278	SER	2.1
1	C	249	GLY	2.1
1	B	161	ASN	2.1
1	C	221	ASP	2.1
1	A	227	LEU	2.1
1	A	294	TYR	2.1
1	A	163(F)	ALA	2.1
1	A	233	GLN	2.1
1	A	251	ALA	2.1
1	B	169	GLN	2.1
1	C	237	ALA	2.1
1	A	184	GLY	2.1
1	C	163(D)	GLU	2.1
1	A	24	SER	2.1
1	A	46	LYS	2.1
1	A	268	GLY	2.1
1	A	303	PHE	2.1
1	C	174	PHE	2.1
1	C	88	LEU	2.1
1	A	235	TYR	2.1
1	C	166	ALA	2.1
1	C	188	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	89	LYS	2.0
1	A	163(B)	SER	2.0
1	A	163(H)	ASN	2.0
1	A	122	THR	2.0
1	A	333	ALA	2.0
1	B	53	ASP	2.0
1	A	293	LYS	2.0
1	A	322	SER	2.0
1	A	192	ALA	2.0
1	C	238	THR	2.0
1	C	171	GLY	2.0
1	C	200	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	D12	A	344	12/12	0.43	0.33	72,72,72,72	0
2	D12	A	345	12/12	0.44	0.30	87,87,87,87	0
2	D12	A	341	12/12	0.55	0.27	64,64,64,64	0
2	D12	A	342	12/12	0.58	0.22	81,81,81,81	0
2	D12	A	348	12/12	0.58	0.34	92,92,92,92	0
2	D12	A	349	12/12	0.67	0.40	94,94,94,94	0
2	D12	A	346	12/12	0.69	0.23	67,67,67,67	0
2	D12	A	347	12/12	0.69	0.29	69,69,69,69	0
2	D12	A	343	12/12	0.74	0.27	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.