



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:51 AM UTC

PDB ID : 1A99 / pdb_00001a99
Title : PUTRESCINE RECEPTOR (POTF) FROM E. COLI
Authors : Vassilyev, D.G.; Tomitori, H.; Kashiwagi, K.; Morikawa, K.; Igarashi, K.
Deposited on : 1998-04-17
Resolution : 2.20 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

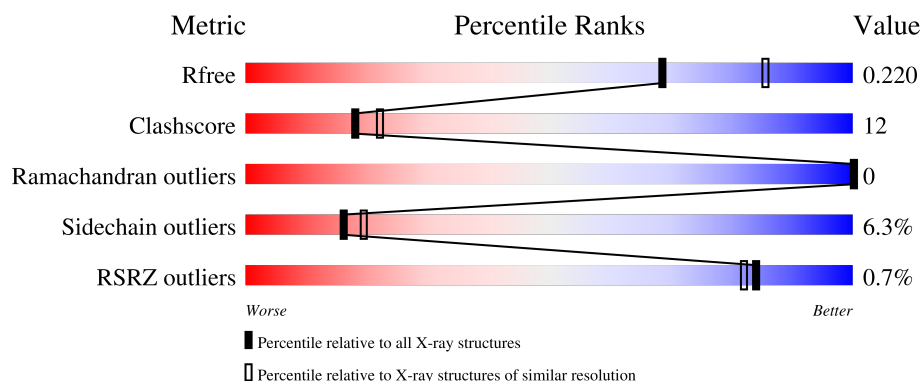
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	344	
1	B	344	
1	C	344	
1	D	344	

2 Entry composition [i](#)

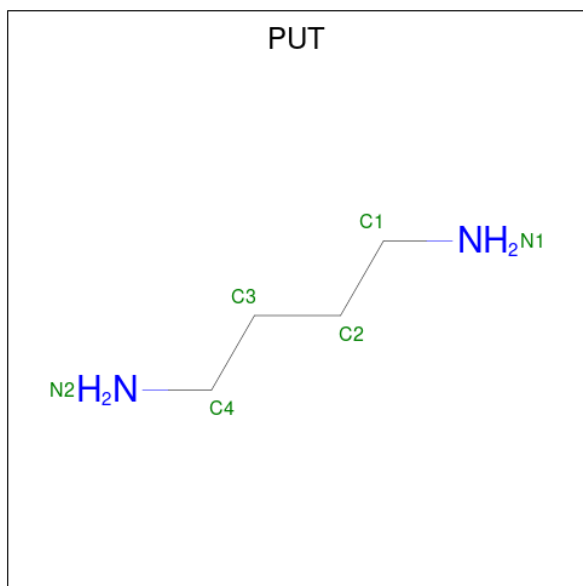
There are 3 unique types of molecules in this entry. The entry contains 11328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTRESCINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2680	1723	445	505	7			
1	B	341	Total	C	N	O	S	0	0	0
			2680	1723	445	505	7			
1	C	341	Total	C	N	O	S	0	0	0
			2680	1723	445	505	7			
1	D	341	Total	C	N	O	S	0	0	0
			2680	1723	445	505	7			

- Molecule 2 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			6	4	2		
2	B	1	Total	C	N	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			6	4	2		
2	D	1	Total	C	N	0	0
			6	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	B	171	Total	O	0	0
			171	171		
3	C	119	Total	O	0	0
			119	119		
3	D	173	Total	O	0	0
			173	173		

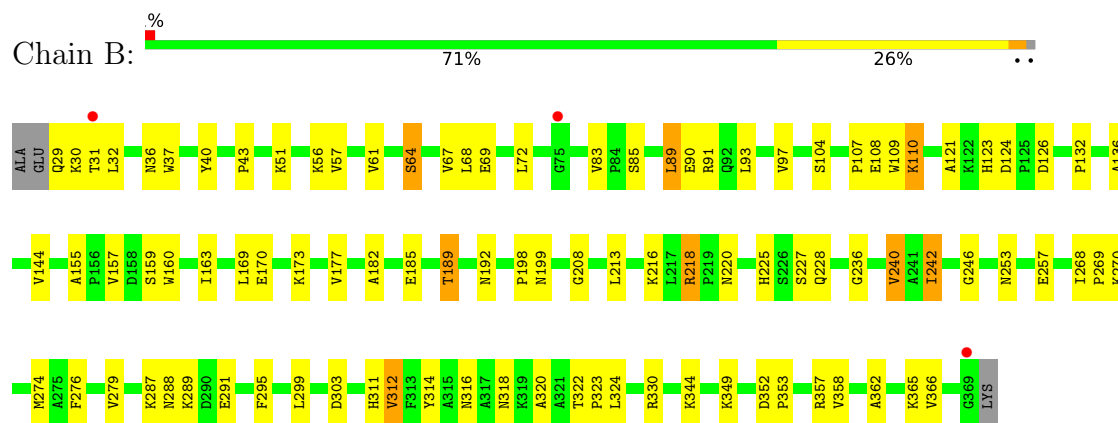
3 Residue-property plots

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.

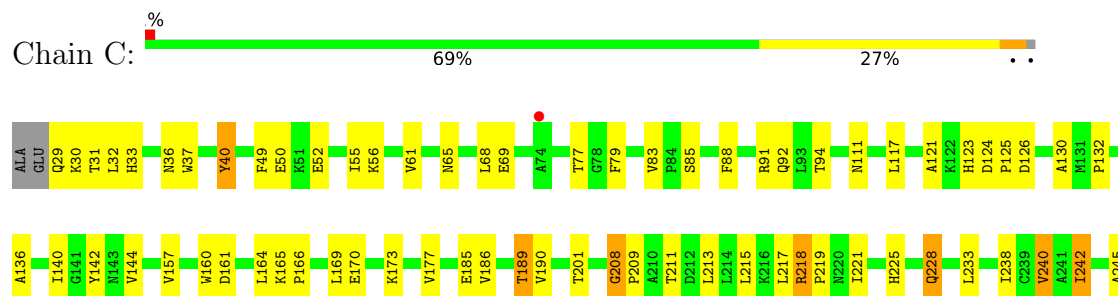
• Molecule 1: PUTRESCINE-BINDING PROTEIN

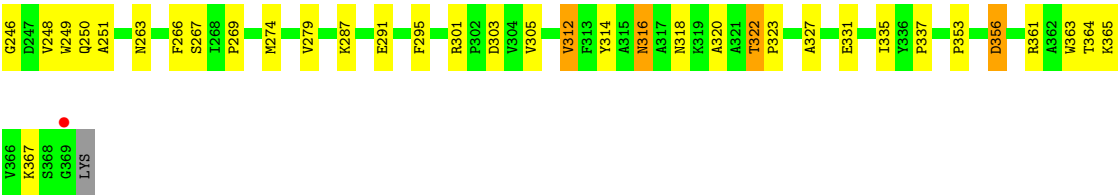


• Molecule 1: PUTRESCINE-BINDING PROTEIN

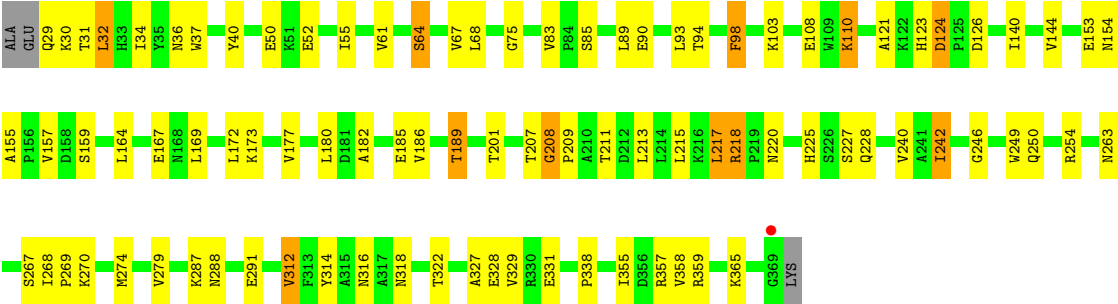


• Molecule 1: PUTRESCINE-BINDING PROTEIN





● Molecule 1: PUTRESCINE-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	269.40Å 82.33Å 93.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.0 (30.00-2.20) 86.4 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	65.73 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.185 , 0.233 0.177 , 0.220	Depositor DCC
R_{free} test set	4619 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.333 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: PUT

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	0.54	0/2748	1.03	9/3740 (0.2%)
1	B	0.60	0/2748	1.02	13/3740 (0.3%)
1	C	0.54	0/2748	0.98	10/3740 (0.3%)
1	D	0.62	0/2748	1.03	11/3740 (0.3%)
All	All	0.58	0/10992	1.01	43/14960 (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	A	242	ILE	N-CA-C	-9.18	95.37	108.58
1	C	242	ILE	N-CA-C	-8.90	95.77	108.58
1	D	242	ILE	N-CA-C	-8.39	95.39	108.23
1	B	242	ILE	N-CA-C	-7.60	96.60	108.23
1	A	106	LEU	CA-C-N	6.97	127.27	119.32
1	A	106	LEU	C-N-CA	6.97	127.27	119.32
1	B	85	SER	N-CA-C	-6.82	101.35	110.55
1	D	85	SER	N-CA-C	-6.71	101.49	110.55
1	A	144	VAL	N-CA-C	6.71	117.40	110.36
1	B	155	ALA	CA-C-N	6.53	128.00	119.84
1	B	155	ALA	C-N-CA	6.53	128.00	119.84
1	B	208	GLY	CA-C-N	6.45	125.95	119.24
1	B	208	GLY	C-N-CA	6.45	125.95	119.24
1	D	144	VAL	N-CA-C	6.43	117.12	110.36
1	B	144	VAL	N-CA-C	6.21	116.88	110.36
1	D	218	ARG	N-CA-C	6.19	121.94	113.77
1	A	208	GLY	CA-C-N	6.12	125.61	119.24
1	A	208	GLY	C-N-CA	6.12	125.61	119.24
1	A	85	SER	N-CA-C	-6.05	102.55	110.53
1	C	144	VAL	N-CA-C	6.02	116.69	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	SER	N-CA-C	-5.97	102.08	110.50
1	B	104	SER	N-CA-C	-5.72	106.14	113.01
1	D	208	GLY	CA-C-N	5.59	125.05	119.24
1	D	208	GLY	C-N-CA	5.59	125.05	119.24
1	C	208	GLY	CA-C-N	5.53	124.99	119.24
1	C	208	GLY	C-N-CA	5.53	124.99	119.24
1	D	124	ASP	CA-C-N	5.50	125.77	119.83
1	D	124	ASP	C-N-CA	5.50	125.77	119.83
1	B	182	ALA	CA-C-N	5.37	126.55	119.84
1	B	182	ALA	C-N-CA	5.37	126.55	119.84
1	D	268	ILE	N-CA-C	-5.34	97.34	108.88
1	C	130	ALA	N-CA-C	5.27	117.83	109.50
1	D	52	GLU	N-CA-C	5.24	117.74	111.71
1	A	141	GLY	N-CA-C	-5.23	102.71	110.71
1	B	268	ILE	N-CA-C	-5.22	97.59	108.88
1	B	218	ARG	N-CA-C	5.22	121.35	109.81
1	D	98	PHE	N-CA-C	5.17	118.17	109.95
1	C	337	PRO	CA-C-N	5.10	125.08	120.03
1	C	337	PRO	C-N-CA	5.10	125.08	120.03
1	C	335	ILE	N-CA-C	-5.10	107.59	111.62
1	A	218	ARG	N-CA-C	5.10	121.07	109.81
1	B	57	VAL	N-CA-C	5.04	115.22	108.17
1	C	140	ILE	N-CA-C	5.01	115.06	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2680	0	2646	62	0
1	B	2680	0	2646	70	0
1	C	2680	0	2646	67	0
1	D	2680	0	2646	63	0
2	A	6	0	12	2	0
2	B	6	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	12	2	0
2	D	6	0	12	3	0
3	A	121	0	0	4	0
3	B	171	0	0	12	0
3	C	119	0	0	6	0
3	D	173	0	0	10	0
All	All	11328	0	10632	260	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 12.

All (260) 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:169:LEU:HD22	1:D:217:LEU:HD13	1.41	0.97
1:D:316:ASN:HD22	1:D:318:ASN:H	1.19	0.90
1:A:185:GLU:O	1:A:189:THR:HG23	1.74	0.87
1:B:316:ASN:HD22	1:B:318:ASN:H	1.24	0.84
1:A:316:ASN:HD22	1:A:318:ASN:H	1.28	0.81
1:A:172:LEU:HD13	1:A:240:VAL:HG21	1.62	0.80
1:A:312:VAL:HG13	1:A:314:TYR:HD2	1.46	0.79
1:D:64:SER:OG	1:D:67:VAL:HG23	1.82	0.79
1:D:312:VAL:HG13	1:D:314:TYR:HD2	1.46	0.79
1:A:218:ARG:O	1:A:218:ARG:HD3	1.82	0.78
1:C:312:VAL:HG13	1:C:314:TYR:HD2	1.49	0.76
1:C:303:ASP:HB2	3:C:765:HOH:O	1.85	0.76
1:C:185:GLU:O	1:C:189:THR:HG23	1.88	0.74
1:B:312:VAL:HG13	1:B:314:TYR:HD1	1.52	0.73
1:C:316:ASN:HD22	1:C:318:ASN:H	1.37	0.71
1:B:108:GLU:HG3	3:B:428:HOH:O	1.92	0.70
1:B:64:SER:OG	1:B:67:VAL:HG23	1.92	0.69
1:D:89:LEU:HD13	1:D:93:LEU:HD23	1.75	0.69
1:D:218:ARG:O	1:D:218:ARG:HD3	1.93	0.68
1:B:225:HIS:CD2	1:B:228:GLN:H	2.12	0.68
1:B:225:HIS:HD2	1:B:227:SER:H	1.42	0.67
1:D:225:HIS:CD2	1:D:228:GLN:H	2.14	0.66
1:D:30:LYS:HA	3:D:951:HOH:O	1.95	0.66
1:A:218:ARG:HD3	1:A:218:ARG:C	2.22	0.64
1:B:185:GLU:HG2	1:B:274:MET:SD	2.38	0.64
1:D:173:LYS:HG3	1:D:220:ASN:HA	1.80	0.64
1:D:185:GLU:O	1:D:189:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ARG:HD2	3:D:872:HOH:O	1.98	0.64
1:D:185:GLU:HG2	1:D:274:MET:SD	2.38	0.64
1:D:164:LEU:HA	1:D:217:LEU:HD11	1.79	0.63
1:B:31:THR:O	1:B:288:ASN:ND2	2.31	0.63
1:B:30:LYS:HG3	3:B:952:HOH:O	1.99	0.63
1:C:160:TRP:HB3	1:C:164:LEU:HD12	1.80	0.62
1:B:72:LEU:HD22	1:B:97:VAL:CG1	2.29	0.62
1:B:357:ARG:HD2	3:B:617:HOH:O	1.99	0.62
1:B:90:GLU:HB2	1:B:123:HIS:HB3	1.81	0.62
1:A:158:ASP:O	1:A:270:LYS:HG2	1.99	0.61
1:B:72:LEU:HD22	1:B:97:VAL:HG11	1.82	0.61
1:A:246:GLY:O	1:A:250:GLN:HG3	2.00	0.61
1:D:31:THR:O	1:D:288:ASN:ND2	2.34	0.61
1:B:110:LYS:HD3	1:B:110:LYS:N	2.16	0.61
1:B:291:GLU:OE1	1:B:291:GLU:N	2.33	0.60
1:D:218:ARG:HD3	1:D:218:ARG:C	2.26	0.60
1:A:159:SER:HB2	1:A:271:GLU:OE2	2.01	0.60
1:C:217:LEU:C	1:C:219:PRO:HD2	2.27	0.60
1:D:225:HIS:HD2	1:D:227:SER:H	1.49	0.59
1:C:177:VAL:HG22	1:C:240:VAL:HG23	1.84	0.59
1:C:218:ARG:HD3	1:C:218:ARG:C	2.26	0.59
1:C:218:ARG:HD3	1:C:218:ARG:O	2.02	0.59
1:A:322:THR:HB	1:A:323:PRO:HD3	1.85	0.59
1:C:33:HIS:HB3	3:C:877:HOH:O	2.03	0.59
1:D:185:GLU:O	1:D:189:THR:CG2	2.50	0.59
1:D:121:ALA:HA	1:D:124:ASP:O	2.03	0.58
1:B:185:GLU:O	1:B:189:THR:CG2	2.52	0.58
1:B:159:SER:HB2	1:B:270:LYS:HE2	1.86	0.58
1:D:215:LEU:HD23	3:D:744:HOH:O	2.04	0.58
1:C:36:ASN:O	1:C:61:VAL:HA	2.04	0.57
1:B:30:LYS:HD2	1:B:291:GLU:OE2	2.05	0.57
1:B:199:ASN:ND2	1:B:349:LYS:HG3	2.20	0.57
1:B:322:THR:HB	1:B:323:PRO:HD3	1.87	0.57
1:B:185:GLU:O	1:B:189:THR:HG23	2.05	0.57
1:D:312:VAL:HG13	1:D:314:TYR:CD2	2.35	0.57
1:D:172:LEU:HD13	1:D:240:VAL:HG21	1.87	0.56
1:D:36:ASN:O	1:D:61:VAL:HA	2.06	0.56
1:A:36:ASN:O	1:A:61:VAL:HA	2.06	0.55
1:B:311:HIS:HB3	3:B:671:HOH:O	2.07	0.55
1:D:103:LYS:HE2	3:D:697:HOH:O	2.05	0.55
1:A:128:LYS:HA	3:A:846:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:HA	1:A:124:ASP:O	2.07	0.55
1:A:196:LYS:HE2	1:A:205:ASP:OD1	2.06	0.55
1:C:88:PHE:O	1:C:92:GLN:HG3	2.07	0.55
1:D:169:LEU:CD2	1:D:217:LEU:HD13	2.26	0.55
1:C:267:SER:O	1:C:269:PRO:HD3	2.07	0.54
1:D:365:LYS:HE3	3:D:703:HOH:O	2.07	0.54
1:D:37:TRP:CE3	2:D:371:PUT:H31	2.43	0.54
1:D:316:ASN:HD22	1:D:318:ASN:N	2.00	0.54
1:D:338:PRO:HD2	3:D:689:HOH:O	2.08	0.54
1:C:218:ARG:HA	1:C:221:ILE:HD12	1.90	0.53
1:B:121:ALA:HA	1:B:124:ASP:O	2.08	0.53
1:C:177:VAL:HG22	1:C:240:VAL:CG2	2.39	0.53
1:B:36:ASN:O	1:B:61:VAL:HA	2.09	0.52
1:B:312:VAL:HG13	1:B:314:TYR:CD1	2.39	0.52
1:A:125:PRO:O	1:A:126:ASP:HB2	2.09	0.52
1:B:246:GLY:HA3	1:B:314:TYR:CE1	2.45	0.52
1:C:185:GLU:CD	1:C:274:MET:HE1	2.34	0.52
1:C:225:HIS:CD2	1:C:228:GLN:H	2.27	0.52
1:B:136:ALA:HB3	1:B:276:PHE:CZ	2.43	0.52
1:B:110:LYS:N	1:B:110:LYS:CD	2.70	0.52
1:B:64:SER:CB	1:B:67:VAL:HG23	2.39	0.52
1:A:359:ARG:HD2	3:A:613:HOH:O	2.10	0.51
1:A:287:LYS:H	1:A:287:LYS:HD3	1.75	0.51
1:D:225:HIS:HD2	1:D:228:GLN:H	1.55	0.51
1:A:142:TYR:OH	1:A:157:VAL:HG11	2.11	0.51
1:B:109:TRP:HB3	1:B:110:LYS:NZ	2.26	0.51
1:C:121:ALA:HA	1:C:124:ASP:O	2.10	0.51
1:D:94:THR:HB	3:D:885:HOH:O	2.09	0.51
1:C:40:TYR:CD1	2:C:371:PUT:H12	2.45	0.50
1:B:173:LYS:HD2	1:B:220:ASN:HA	1.92	0.50
1:D:90:GLU:OE1	1:D:123:HIS:HD2	1.94	0.50
1:D:169:LEU:HD11	1:D:177:VAL:HG11	1.94	0.50
1:B:36:ASN:ND2	1:B:37:TRP:H	2.09	0.50
1:A:330:ARG:HD2	3:A:980:HOH:O	2.12	0.49
1:D:250:GLN:O	1:D:254:ARG:HG3	2.11	0.49
1:C:185:GLU:HG2	1:C:274:MET:SD	2.52	0.49
1:A:106:LEU:HA	1:A:297:ASN:HD21	1.77	0.49
1:C:322:THR:HG23	1:C:323:PRO:HD3	1.93	0.49
1:D:211:THR:HG22	1:D:215:LEU:CD1	2.42	0.49
1:C:77:THR:HB	1:C:79:PHE:CD2	2.48	0.49
1:A:256:LYS:O	1:A:259:LYS:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:HB3	1:C:88:PHE:CE2	2.48	0.49
1:D:316:ASN:ND2	1:D:318:ASN:H	2.00	0.49
1:B:323:PRO:HD3	3:B:967:HOH:O	2.12	0.49
1:A:307:HIS:CE1	1:A:311:HIS:CE1	3.01	0.48
1:B:236:GLY:HA2	3:B:406:HOH:O	2.13	0.48
1:C:161:ASP:O	1:C:165:LYS:HB2	2.13	0.48
1:C:49:PHE:CE1	1:C:295:PHE:HA	2.48	0.48
1:C:123:HIS:HE1	3:C:862:HOH:O	1.96	0.48
1:C:363:TRP:NE1	1:C:367:LYS:HE2	2.28	0.48
1:D:32:LEU:HD13	1:D:34:ILE:HD11	1.95	0.48
1:D:37:TRP:CD2	2:D:371:PUT:H31	2.49	0.48
1:B:192:ASN:HB2	1:B:198:PRO:HG3	1.96	0.48
1:B:322:THR:HG22	1:B:330:ARG:HD3	1.95	0.48
1:A:316:ASN:HD22	1:A:318:ASN:N	2.04	0.48
1:A:312:VAL:CG1	1:A:314:TYR:HD2	2.21	0.48
1:D:110:LYS:HZ3	1:D:110:LYS:HB2	1.79	0.48
1:C:69:GLU:OE2	1:C:91:ARG:HD2	2.13	0.47
1:D:207:THR:HG23	1:D:358:VAL:HG13	1.95	0.47
1:D:291:GLU:OE1	1:D:291:GLU:N	2.40	0.47
1:C:136:ALA:HB1	1:C:245:ALA:HB3	1.97	0.47
1:C:36:ASN:ND2	1:C:83:VAL:HG21	2.30	0.47
1:C:312:VAL:CG1	1:C:314:TYR:HD2	2.21	0.47
1:D:267:SER:O	1:D:269:PRO:HD3	2.14	0.47
1:A:36:ASN:ND2	1:A:83:VAL:HG21	2.30	0.47
1:B:225:HIS:HD2	1:B:228:GLN:H	1.58	0.47
1:C:225:HIS:CD2	1:C:228:GLN:HB2	2.50	0.47
1:A:42:ALA:HB3	1:A:45:THR:OG1	2.14	0.47
1:C:327:ALA:O	1:C:331:GLU:HB2	2.15	0.47
1:D:246:GLY:O	1:D:250:GLN:HG3	2.15	0.47
1:B:110:LYS:CD	1:B:110:LYS:H	2.28	0.47
1:B:43:PRO:HD3	3:B:801:HOH:O	2.14	0.47
1:A:332:ASN:HB3	1:A:335:ILE:HD12	1.97	0.46
1:C:37:TRP:CD2	2:C:371:PUT:H31	2.50	0.46
1:C:246:GLY:O	1:C:250:GLN:HG3	2.14	0.46
1:B:316:ASN:HD22	1:B:318:ASN:N	2.02	0.46
1:C:166:PRO:O	1:C:170:GLU:HG3	2.15	0.46
1:D:90:GLU:HB2	1:D:123:HIS:HB3	1.98	0.46
1:C:215:LEU:HA	1:C:215:LEU:HD23	1.81	0.46
1:C:225:HIS:HD2	1:C:228:GLN:H	1.63	0.46
1:A:207:THR:HG23	1:A:358:VAL:HG13	1.97	0.46
1:D:246:GLY:HA3	1:D:314:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:HB3	1:A:82:VAL:HG12	1.97	0.46
1:A:201:THR:O	1:A:355:ILE:HD11	2.16	0.45
1:C:316:ASN:HD22	1:C:318:ASN:N	2.11	0.45
1:A:236:GLY:HA2	3:A:746:HOH:O	2.17	0.45
1:D:37:TRP:HB3	2:D:371:PUT:H11	1.99	0.45
1:C:353:PRO:HA	1:C:356:ASP:HB2	1.98	0.45
1:A:185:GLU:HG2	1:A:274:MET:SD	2.56	0.45
1:C:111:ASN:HB3	1:C:318:ASN:OD1	2.16	0.45
1:C:248:VAL:HG21	1:C:266:PHE:HD1	1.82	0.45
1:D:50:GLU:HG2	1:D:55:ILE:O	2.16	0.45
1:D:108:GLU:HB2	3:D:414:HOH:O	2.17	0.45
1:D:159:SER:HB2	1:D:270:LYS:NZ	2.32	0.45
1:C:30:LYS:HB3	1:C:291:GLU:OE2	2.16	0.45
1:B:31:THR:HG23	1:B:56:LYS:CE	2.46	0.45
1:D:357:ARG:NH2	3:D:763:HOH:O	2.49	0.45
1:B:36:ASN:ND2	1:B:83:VAL:HG21	2.32	0.45
1:B:289:LYS:HB3	1:B:289:LYS:HE2	1.82	0.45
1:C:185:GLU:O	1:C:189:THR:CG2	2.60	0.45
1:C:363:TRP:CD1	1:C:367:LYS:HE2	2.51	0.45
1:C:246:GLY:HA3	1:C:314:TYR:CE2	2.52	0.45
1:D:89:LEU:HD22	1:D:98:PHE:CE2	2.51	0.44
1:A:287:LYS:HD3	1:A:287:LYS:N	2.31	0.44
1:A:289:LYS:HB3	1:A:289:LYS:HE2	1.82	0.44
1:B:276:PHE:CE2	2:B:371:PUT:H41	2.51	0.44
1:B:303:ASP:HA	1:B:324:LEU:HD23	1.99	0.44
1:A:107:PRO:HD2	1:A:297:ASN:OD1	2.16	0.44
1:A:314:TYR:OH	2:A:371:PUT:H21	2.18	0.44
1:B:177:VAL:HG22	1:B:240:VAL:CG2	2.47	0.44
1:C:36:ASN:HD22	1:C:83:VAL:HB	1.82	0.44
1:A:130:ALA:HB1	1:A:279:VAL:HB	1.99	0.44
1:A:148:LYS:CA	1:A:148:LYS:HE3	2.48	0.44
1:B:169:LEU:HD11	1:B:177:VAL:HG11	2.00	0.44
1:C:186:VAL:O	1:C:190:VAL:HG23	2.18	0.44
1:C:316:ASN:ND2	1:C:318:ASN:H	2.10	0.44
1:C:320:ALA:O	1:C:323:PRO:HD2	2.17	0.44
1:A:169:LEU:HD22	1:A:217:LEU:HD22	1.99	0.44
1:A:267:SER:O	1:A:269:PRO:HD3	2.18	0.44
1:B:362:ALA:O	1:B:366:VAL:HG23	2.18	0.44
1:C:117:LEU:HD23	1:C:132:PRO:HG2	1.99	0.44
1:A:56:LYS:HD3	1:A:57:VAL:N	2.32	0.44
1:B:90:GLU:OE1	1:B:123:HIS:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD11	1:C:177:VAL:HG11	2.00	0.44
1:D:36:ASN:ND2	1:D:83:VAL:HG21	2.33	0.44
1:A:36:ASN:ND2	1:A:37:TRP:H	2.14	0.43
1:B:365:LYS:NZ	3:B:418:HOH:O	2.51	0.43
1:C:83:VAL:HA	1:C:279:VAL:O	2.18	0.43
1:D:182:ALA:O	1:D:186:VAL:HG23	2.18	0.43
1:C:248:VAL:O	1:C:251:ALA:HB3	2.17	0.43
1:A:256:LYS:HB2	1:A:256:LYS:HE3	1.86	0.43
1:B:107:PRO:O	1:B:110:LYS:HE2	2.18	0.43
1:D:110:LYS:HB2	1:D:110:LYS:NZ	2.33	0.43
1:A:302:PRO:HA	1:A:321:ALA:HB2	2.01	0.43
1:A:320:ALA:O	1:A:323:PRO:HD2	2.19	0.43
1:D:75:GLY:HA2	3:D:756:HOH:O	2.19	0.43
1:C:52:GLU:HG2	3:C:820:HOH:O	2.19	0.43
1:A:217:LEU:C	1:A:219:PRO:HD2	2.44	0.43
1:B:64:SER:HB2	3:B:812:HOH:O	2.17	0.43
1:A:185:GLU:O	1:A:189:THR:CG2	2.57	0.43
1:B:257:GLU:HG3	3:B:833:HOH:O	2.18	0.43
1:B:295:PHE:CE2	1:B:299:LEU:HD11	2.54	0.42
1:C:125:PRO:O	1:C:126:ASP:HB2	2.20	0.42
1:C:233:LEU:HG	1:C:238:ILE:HD11	2.00	0.42
1:B:163:ILE:HD13	1:B:242:ILE:HG13	2.01	0.42
1:B:311:HIS:HB3	3:B:801:HOH:O	2.19	0.42
1:D:83:VAL:HA	1:D:279:VAL:O	2.18	0.42
1:D:327:ALA:O	1:D:331:GLU:HB2	2.18	0.42
1:A:225:HIS:HD2	1:A:227:SER:H	1.67	0.42
1:B:218:ARG:HD3	1:B:366:VAL:O	2.19	0.42
1:B:320:ALA:O	1:B:323:PRO:HD2	2.19	0.42
1:A:83:VAL:HA	1:A:279:VAL:O	2.20	0.42
1:C:211:THR:HG21	1:C:365:LYS:HE3	2.02	0.42
1:B:253:ASN:O	1:B:257:GLU:HG2	2.20	0.42
1:D:154:ASN:O	1:D:155:ALA:C	2.63	0.42
1:A:65:ASN:HB3	1:A:88:PHE:CE2	2.55	0.42
1:A:140:ILE:HG21	1:A:162:LEU:HD23	2.02	0.42
1:A:250:GLN:O	1:A:254:ARG:HG3	2.19	0.42
1:A:165:LYS:HG2	1:A:167:GLU:HG2	2.02	0.41
1:A:312:VAL:HG13	1:A:314:TYR:CD2	2.38	0.41
1:B:160:TRP:CE2	1:B:269:PRO:HG2	2.54	0.41
1:A:133:TYR:CD2	1:A:134:MET:HG2	2.55	0.41
1:A:154:ASN:O	1:A:155:ALA:C	2.64	0.41
1:B:314:TYR:OH	2:B:371:PUT:H21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TRP:CD2	2:B:371:PUT:H31	2.55	0.41
1:B:132:PRO:HA	1:B:279:VAL:HG12	2.02	0.41
1:A:148:LYS:HE3	1:A:148:LYS:HA	2.02	0.41
1:D:328:GLU:HG3	1:D:329:VAL:N	2.35	0.41
1:C:208:GLY:HA3	1:C:209:PRO:HD2	1.91	0.41
1:A:52:GLU:HG3	1:B:107:PRO:HG3	2.02	0.41
1:B:64:SER:HB3	1:B:67:VAL:HG23	2.02	0.41
1:B:69:GLU:OE2	1:B:91:ARG:HD2	2.21	0.41
1:B:199:ASN:HB2	3:B:814:HOH:O	2.21	0.41
1:C:249:TRP:CZ2	1:C:266:PHE:HB3	2.56	0.41
1:C:301:ARG:HD2	3:C:773:HOH:O	2.20	0.41
1:D:140:ILE:HD12	1:D:269:PRO:HG3	2.01	0.41
1:A:40:TYR:CD1	2:A:371:PUT:H12	2.56	0.41
1:B:352:ASP:HB2	1:B:353:PRO:CD	2.51	0.41
1:C:142:TYR:OH	1:C:157:VAL:HG11	2.21	0.41
1:C:263:ASN:HB2	3:C:931:HOH:O	2.21	0.41
1:C:312:VAL:HG13	1:C:314:TYR:CD2	2.41	0.41
1:D:180:LEU:HG	1:D:242:ILE:O	2.21	0.41
1:D:201:THR:O	1:D:355:ILE:HD11	2.21	0.41
1:A:35:TYR:CD2	1:A:68:LEU:HD23	2.55	0.41
1:D:208:GLY:HA3	1:D:209:PRO:HD3	1.98	0.40
1:A:103:LYS:HE2	1:A:109:TRP:CZ2	2.56	0.40
1:C:31:THR:HA	1:C:56:LYS:O	2.20	0.40
1:C:50:GLU:HG2	1:C:55:ILE:O	2.21	0.40
1:C:185:GLU:HG2	1:C:274:MET:HE1	2.04	0.40
1:A:107:PRO:HB3	1:B:51:LYS:HE3	2.03	0.40
1:B:89:LEU:HD13	1:B:93:LEU:HD23	2.04	0.40
1:D:249:TRP:HA	1:D:249:TRP:CE3	2.56	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	339/344 (98%)	332 (98%)	7 (2%)	0	100	100
1	B	339/344 (98%)	329 (97%)	10 (3%)	0	100	100
1	C	339/344 (98%)	329 (97%)	10 (3%)	0	100	100
1	D	339/344 (98%)	331 (98%)	8 (2%)	0	100	100
All	All	1356/1376 (98%)	1321 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	288/290 (99%)	271 (94%)	17 (6%)	18	22
1	B	288/290 (99%)	270 (94%)	18 (6%)	16	19
1	C	288/290 (99%)	267 (93%)	21 (7%)	13	15
1	D	288/290 (99%)	271 (94%)	17 (6%)	18	22
All	All	1152/1160 (99%)	1079 (94%)	73 (6%)	16	19

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	32	LEU
1	A	40	TYR
1	A	68	LEU
1	A	89	LEU
1	A	115	GLU
1	A	148	LYS
1	A	157	VAL
1	A	165	LYS
1	A	189	THR
1	A	213	LEU
1	A	228	GLN
1	A	287	LYS

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Mol	Chain	Res	Type
1	A	305	VAL
1	A	312	VAL
1	A	349	LYS
1	A	352	ASP
1	B	29	GLN
1	B	32	LEU
1	B	40	TYR
1	B	64	SER
1	B	68	LEU
1	B	89	LEU
1	B	110	LYS
1	B	126	ASP
1	B	157	VAL
1	B	170	GLU
1	B	189	THR
1	B	213	LEU
1	B	216	LYS
1	B	240	VAL
1	B	287	LYS
1	B	312	VAL
1	B	344	LYS
1	B	358	VAL
1	C	29	GLN
1	C	32	LEU
1	C	40	TYR
1	C	68	LEU
1	C	94	THR
1	C	173	LYS
1	C	189	THR
1	C	201	THR
1	C	213	LEU
1	C	218	ARG
1	C	228	GLN
1	C	240	VAL
1	C	242	ILE
1	C	287	LYS
1	C	305	VAL
1	C	312	VAL
1	C	316	ASN
1	C	322	THR
1	C	356	ASP
1	C	361	ARG

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Mol	Chain	Res	Type
1	C	364	THR
1	D	29	GLN
1	D	32	LEU
1	D	40	TYR
1	D	64	SER
1	D	68	LEU
1	D	110	LYS
1	D	126	ASP
1	D	153	GLU
1	D	157	VAL
1	D	167	GLU
1	D	189	THR
1	D	213	LEU
1	D	217	LEU
1	D	263	ASN
1	D	287	LYS
1	D	312	VAL
1	D	322	THR

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

Mol	Chain	Res	Type
1	A	33	HIS
1	A	36	ASN
1	A	123	HIS
1	A	225	HIS
1	A	228	GLN
1	A	263	ASN
1	A	311	HIS
1	A	316	ASN
1	B	36	ASN
1	B	123	HIS
1	B	127	ASN
1	B	225	HIS
1	B	263	ASN
1	B	294	GLN
1	B	316	ASN
1	C	36	ASN
1	C	99	GLN
1	C	123	HIS
1	C	168	ASN
1	C	225	HIS

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Mol	Chain	Res	Type
1	C	235	ASN
1	C	316	ASN
1	D	36	ASN
1	D	123	HIS
1	D	127	ASN
1	D	225	HIS
1	D	235	ASN
1	D	316	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PUT	B	371	-	5,5,5	0.45	0	4,4,4	0.26	0
2	PUT	C	371	-	5,5,5	0.42	0	4,4,4	0.25	0
2	PUT	D	371	-	5,5,5	0.50	0	4,4,4	0.25	0
2	PUT	A	371	-	5,5,5	0.37	0	4,4,4	0.17	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	PUT	B	371	-	-	0/3/3/3	-
2	PUT	C	371	-	-	0/3/3/3	-
2	PUT	D	371	-	-	0/3/3/3	-
2	PUT	A	371	-	-	0/3/3/3	-

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.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	371	PUT	3	0
2	C	371	PUT	2	0
2	D	371	PUT	3	0
2	A	371	PUT	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/344 (99%)	-0.19	3 (0%) 81 79	21, 39, 65, 91	0
1	B	341/344 (99%)	-0.46	3 (0%) 81 79	16, 30, 54, 86	0
1	C	341/344 (99%)	-0.17	2 (0%) 85 83	21, 40, 66, 92	0
1	D	341/344 (99%)	-0.47	1 (0%) 90 88	12, 29, 52, 90	0
All	All	1364/1376 (99%)	-0.33	9 (0%) 84 82	12, 34, 63, 92	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	GLY	3.8
1	B	369	GLY	3.4
1	C	369	GLY	3.1
1	A	369	GLY	2.9
1	A	287	LYS	2.3
1	B	75	GLY	2.3
1	C	74	ALA	2.3
1	A	361	ARG	2.2
1	B	31	THR	2.1

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($\text{\AA}^2$)	Q<0.9
2	PUT	B	371	6/6	0.95	0.06	19,20,21,21	0
2	PUT	A	371	6/6	0.97	0.05	17,21,23,25	0
2	PUT	C	371	6/6	0.97	0.06	16,20,22,23	0
2	PUT	D	371	6/6	0.97	0.05	15,23,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.