



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:07 AM EDT

PDB ID : 2JHE / pdb_00002jhe
Title : N-terminal domain of TyrR transcription factor (residues 1 - 190)
Authors : Verger, D.; Carr, P.D.; Kwok, T.; Ollis, D.L.
Deposited on : 2007-02-21
Resolution : 2.30 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

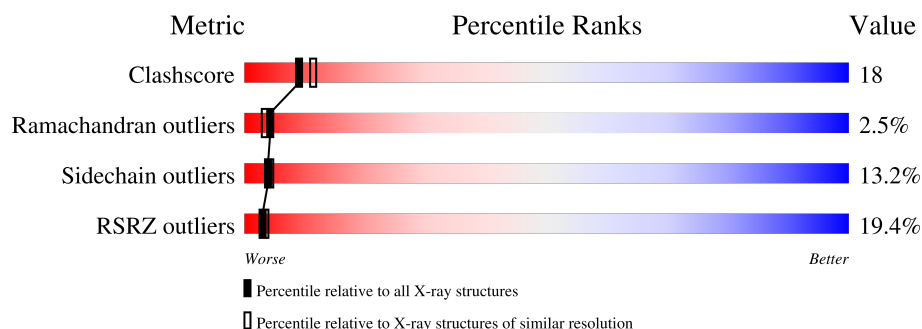
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	190	16% 61% 31% 7% ..
1	B	190	15% 67% 25% 7% ..
1	C	190	19% 64% 24% 8% ..
1	D	190	26% 66% 26% 7% ..

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
3	PG4	C	1189	-	-	X	-

2 Entry composition [i](#)

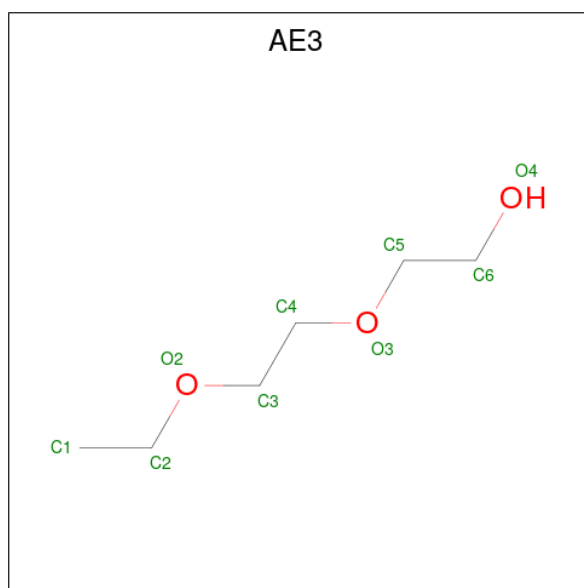
There are 5 unique types of molecules in this entry. The entry contains 5900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSCRIPTION REGULATOR TYRR.

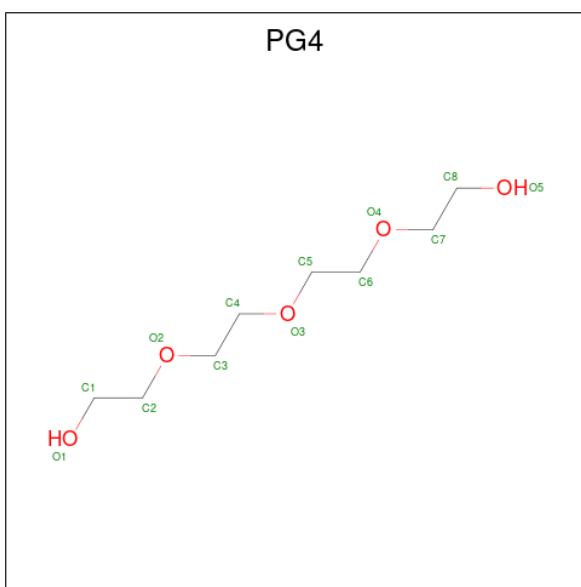
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1398	885	247	257	9			
1	B	189	Total	C	N	O	S	0	0	0
			1468	927	257	275	9			
1	C	187	Total	C	N	O	S	0	0	0
			1433	901	254	269	9			
1	D	189	Total	C	N	O	S	0	0	0
			1417	892	249	267	9			

- Molecule 2 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: C₆H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		
3	C	1	Total	C	O	0	0
			12	8	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

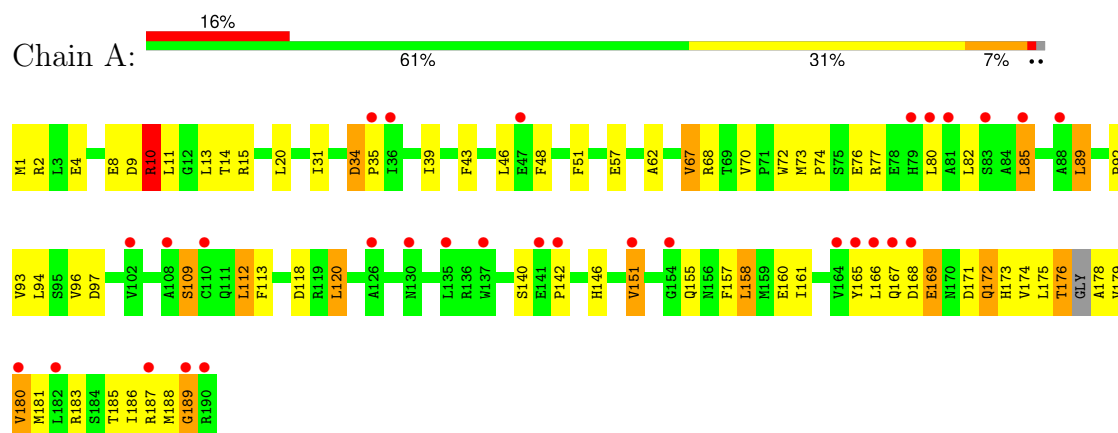
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total 43	O 43	0	0
5	B	48	Total 48	O 48	0	0
5	C	35	Total 35	O 35	0	0
5	D	20	Total 20	O 20	0	0

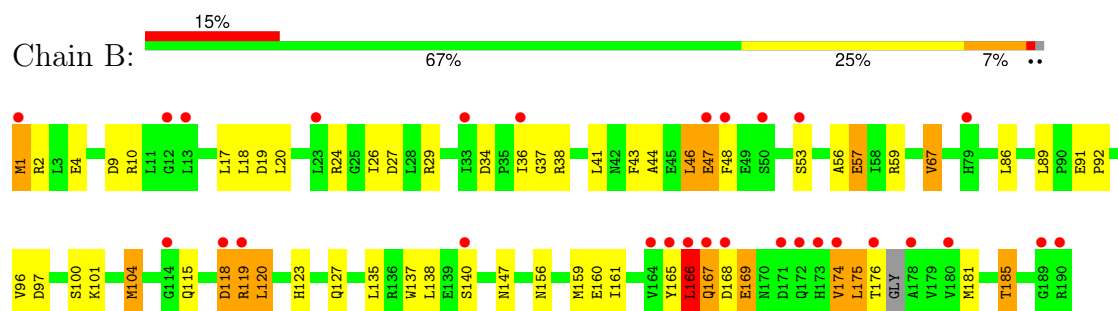
3 Residue-property plots

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.

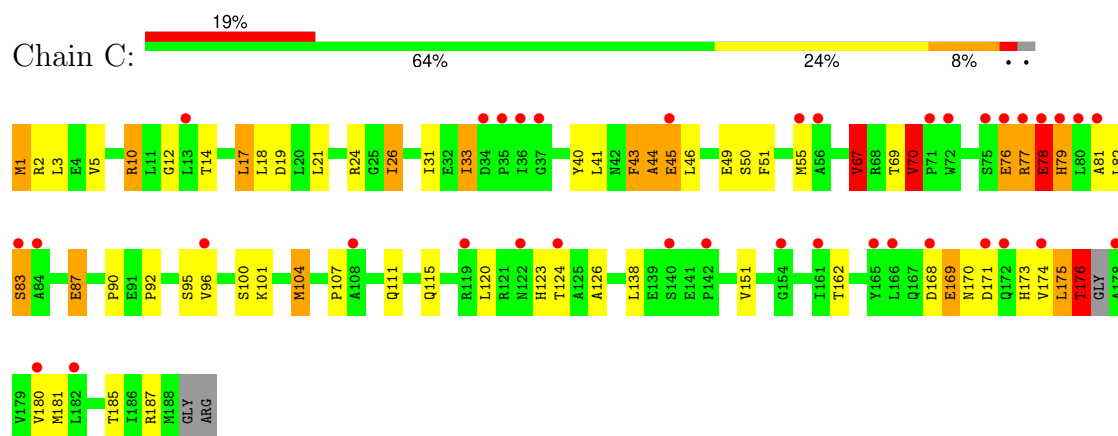
• Molecule 1: TRANSCRIPTION REGULATOR TYRR



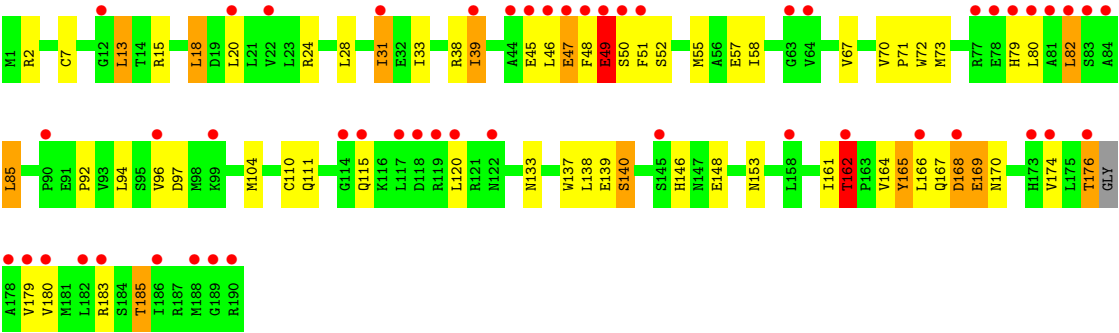
• Molecule 1: TRANSCRIPTION REGULATOR TYRR



• Molecule 1: TRANSCRIPTION REGULATOR TYRR



● Molecule 1: TRANSCRIPTION REGULATOR TYRR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.46Å 72.01Å 96.81Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	24.40 – 2.30 24.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (24.40-2.30) 98.1 (24.40-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.317 0.249 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5900	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AE3, PG4

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	1.43	1/1421 (0.1%)	1.17	8/1935 (0.4%)
1	B	1.26	3/1494 (0.2%)	1.26	5/2028 (0.2%)
1	C	1.04	1/1456 (0.1%)	1.19	6/1977 (0.3%)
1	D	1.05	4/1441 (0.3%)	1.23	7/1962 (0.4%)
All	All	1.20	9/5812 (0.2%)	1.21	26/7902 (0.3%)

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	B	0	1
1	C	0	2
1	D	0	3
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	THR	C-N	37.52	1.86	1.33
1	B	176	THR	C-N	22.20	1.63	1.34
1	D	176	THR	C-N	-10.28	1.20	1.33
1	D	185	THR	CA-CB	7.79	1.65	1.53
1	B	174	VAL	CA-CB	6.67	1.62	1.54
1	B	56	ALA	CA-CB	5.43	1.61	1.53
1	C	33	ILE	CA-CB	5.38	1.60	1.54
1	D	179	VAL	CA-CB	5.28	1.60	1.54
1	D	39	ILE	CA-CB	5.01	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	THR	O-C-N	-13.09	105.14	123.07
1	D	50	SER	N-CA-C	-8.92	100.40	111.11
1	B	176	THR	CA-C-N	7.93	131.96	120.38
1	B	176	THR	C-N-CA	7.93	131.96	120.38
1	D	166	LEU	N-CA-C	-7.52	101.62	111.02
1	A	89	LEU	CA-C-N	6.91	126.61	119.56
1	A	89	LEU	C-N-CA	6.91	126.61	119.56
1	B	67	VAL	CB-CA-C	-6.79	98.74	111.30
1	C	79	HIS	N-CA-C	-6.70	104.97	113.01
1	C	176	THR	CA-C-N	6.36	133.68	121.54
1	C	176	THR	C-N-CA	6.36	133.68	121.54
1	D	162	THR	CA-C-N	6.14	126.46	119.83
1	D	162	THR	C-N-CA	6.14	126.46	119.83
1	C	70	VAL	CA-C-N	-6.12	112.19	119.84
1	C	70	VAL	C-N-CA	-6.12	112.19	119.84
1	D	165	TYR	N-CA-C	5.95	119.15	110.17
1	D	140	SER	N-CA-C	-5.73	106.29	113.28
1	C	67	VAL	CB-CA-C	-5.53	101.99	110.50
1	A	10	ARG	N-CA-C	5.45	118.34	109.24
1	A	176	THR	O-C-N	-5.41	115.39	122.59
1	A	142	PRO	N-CA-C	5.30	119.52	111.15
1	A	34	ASP	CA-C-N	5.28	126.43	119.84
1	A	34	ASP	C-N-CA	5.28	126.43	119.84
1	A	67	VAL	CB-CA-C	-5.21	101.38	110.71
1	B	100	SER	N-CA-C	5.19	119.20	112.86
1	D	185	THR	CB-CA-C	5.10	119.52	110.85

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	LEU	Peptide
1	C	176	THR	Mainchain
1	C	78	GLU	Peptide
1	D	165	TYR	Peptide
1	D	176	THR	Mainchain
1	D	49	GLU	Peptide

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	1398	0	1329	61	0
1	B	1468	0	1423	44	2
1	C	1433	0	1389	76	1
1	D	1417	0	1343	41	1
2	A	9	0	14	1	0
3	A	12	0	15	5	0
3	C	12	0	15	9	0
4	B	5	0	0	0	0
5	A	43	0	0	0	0
5	B	48	0	0	2	0
5	C	35	0	0	2	0
5	D	20	0	0	0	0
All	All	5900	0	5528	208	2

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 18.

All (208) 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:C:176:THR:CG2	1:C:180:VAL:HG23	1.31	1.54
1:C:176:THR:CG2	1:C:180:VAL:CG2	1.94	1.43
1:C:176:THR:HG21	1:C:180:VAL:CG2	1.54	1.33
1:A:176:THR:C	1:A:178:ALA:N	1.86	1.33
1:B:1:MET:CE	1:B:46:LEU:HB2	1.72	1.19
1:B:1:MET:HE1	1:B:46:LEU:CB	1.74	1.16
1:C:14:THR:H	3:C:1189:PG4:H42	1.12	1.14
1:C:176:THR:HG23	1:C:180:VAL:HG23	1.15	1.11
1:D:96:VAL:O	1:D:169:GLU:HB2	1.49	1.09
1:C:14:THR:HB	3:C:1189:PG4:H31	1.31	1.06
1:A:94:LEU:HD12	1:A:172:GLN:HE22	1.21	1.02
1:B:96:VAL:O	1:B:169:GLU:CB	2.09	1.00
1:C:176:THR:HG21	1:C:180:VAL:HG23	1.03	0.98
1:C:176:THR:CG2	1:C:180:VAL:HG21	1.95	0.95
1:C:10:ARG:O	3:C:1189:PG4:H51	1.69	0.92
1:C:176:THR:HG23	1:C:180:VAL:CG2	1.79	0.92
1:C:83:SER:O	1:C:87:GLU:HG2	1.69	0.91
1:C:176:THR:HG21	1:C:180:VAL:HG21	1.51	0.89
1:B:115:GLN:HE22	1:B:123:HIS:CE1	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PRO:HB2	1:B:174:VAL:HG22	1.55	0.86
1:A:94:LEU:CD1	1:A:172:GLN:HE22	1.90	0.84
1:D:180:VAL:HG22	1:D:183:ARG:HH12	1.42	0.84
1:A:94:LEU:O	1:A:172:GLN:NE2	2.11	0.84
1:C:92:PRO:HB2	1:C:174:VAL:CG2	2.08	0.84
1:D:168:ASP:O	1:D:169:GLU:HB3	1.77	0.83
1:D:92:PRO:HB2	1:D:174:VAL:HG22	1.61	0.82
1:C:3:LEU:HD21	1:C:51:PHE:HE1	1.44	0.82
1:D:49:GLU:HG2	1:D:49:GLU:O	1.81	0.81
1:C:90:PRO:HD3	1:D:162:THR:HG21	1.62	0.81
1:C:92:PRO:HB2	1:C:174:VAL:HG22	1.61	0.81
1:C:3:LEU:HD21	1:C:51:PHE:CE1	2.18	0.79
1:A:94:LEU:HD12	1:A:172:GLN:NE2	1.97	0.79
1:C:181:MET:O	1:C:185:THR:HG23	1.82	0.78
1:C:78:GLU:HA	1:C:81:ALA:H	1.48	0.78
1:A:2:ARG:HD2	1:A:72:TRP:HA	1.65	0.76
1:A:160:GLU:O	1:A:172:GLN:HB2	1.84	0.76
1:C:176:THR:HG23	1:C:180:VAL:CB	2.14	0.76
1:A:94:LEU:CD1	1:A:172:GLN:NE2	2.49	0.75
1:B:118:ASP:HB2	5:B:2028:HOH:O	1.85	0.75
1:B:20:LEU:HD11	1:B:57:GLU:OE1	1.86	0.74
1:A:2:ARG:HD3	1:A:76:GLU:OE1	1.88	0.74
1:A:158:LEU:HD22	1:A:181:MET:HE1	1.69	0.74
1:C:115:GLN:HE22	1:C:123:HIS:CD2	2.07	0.73
1:A:157:PHE:CD2	1:A:174:VAL:HG12	2.24	0.72
1:C:45:GLU:O	1:C:45:GLU:HG3	1.88	0.72
1:D:28:LEU:HD11	1:D:31:ILE:HG22	1.71	0.72
1:A:109:SER:O	1:A:113:PHE:HD2	1.72	0.71
1:D:47:GLU:C	1:D:49:GLU:H	1.97	0.71
1:C:33:ILE:HD13	1:D:28:LEU:HD23	1.73	0.71
1:A:173:HIS:NE2	1:B:89:LEU:HD22	2.07	0.70
1:D:31:ILE:HD11	1:D:33:ILE:HG13	1.74	0.69
1:C:14:THR:H	3:C:1189:PG4:C4	2.00	0.69
1:A:96:VAL:O	1:A:169:GLU:CB	2.42	0.68
1:C:10:ARG:HB3	1:C:10:ARG:HH11	1.58	0.68
1:D:13:LEU:HD13	1:D:39:ILE:HD12	1.75	0.67
1:B:119:ARG:NH2	5:B:2029:HOH:O	2.27	0.67
1:D:51:PHE:O	1:D:55:MET:HG2	1.95	0.67
1:C:96:VAL:O	1:C:169:GLU:CB	2.42	0.67
1:D:31:ILE:CD1	1:D:39:ILE:HG23	2.25	0.67
1:B:86:LEU:HD23	1:B:104:MET:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD12	1:A:94:LEU:C	2.21	0.65
1:A:94:LEU:HD12	1:A:94:LEU:O	1.97	0.65
1:B:1:MET:CE	1:B:43:PHE:HE1	2.09	0.65
1:D:47:GLU:O	1:D:49:GLU:N	2.30	0.64
1:B:1:MET:HE2	1:B:43:PHE:HE1	1.62	0.64
1:B:115:GLN:HE22	1:B:123:HIS:HE1	1.46	0.63
1:C:79:HIS:HB2	1:D:79:HIS:HA	1.80	0.63
1:A:180:VAL:HG11	3:A:1192:PG4:H22	1.82	0.62
1:C:78:GLU:N	1:C:78:GLU:OE1	2.33	0.62
1:A:10:ARG:CG	1:A:13:LEU:HD12	2.29	0.61
1:A:180:VAL:HG11	3:A:1192:PG4:C2	2.30	0.61
1:D:180:VAL:HG22	1:D:183:ARG:NH1	2.12	0.61
1:C:12:GLY:H	3:C:1189:PG4:C1	2.14	0.61
1:C:173:HIS:CD2	5:C:2034:HOH:O	2.52	0.61
1:A:157:PHE:CD2	1:A:174:VAL:CG1	2.83	0.61
3:A:1192:PG4:H42	1:B:160:GLU:OE2	2.01	0.61
1:D:168:ASP:O	1:D:169:GLU:CB	2.49	0.61
1:C:51:PHE:CZ	1:C:55:MET:SD	2.94	0.60
1:C:175:LEU:HB3	1:C:181:MET:HE2	1.82	0.60
1:C:14:THR:N	3:C:1189:PG4:H42	1.98	0.60
1:A:173:HIS:CE1	1:B:89:LEU:HD22	2.37	0.59
1:C:10:ARG:HH11	1:C:10:ARG:CB	2.15	0.59
1:A:14:THR:HG22	1:B:18:LEU:HD21	1.85	0.59
1:C:77:ARG:HD3	1:C:78:GLU:HB2	1.85	0.58
1:A:72:TRP:NE1	1:A:77:ARG:HG3	2.17	0.58
1:D:137:TRP:O	1:D:140:SER:HB3	2.03	0.58
1:A:2:ARG:CD	1:A:76:GLU:OE1	2.51	0.58
1:A:113:PHE:HB2	1:A:120:LEU:HD11	1.86	0.57
1:C:10:ARG:HH11	1:C:10:ARG:CG	2.16	0.57
1:C:82:LEU:HB3	1:D:82:LEU:HD23	1.87	0.57
1:C:5:VAL:HG22	1:C:67:VAL:HG13	1.87	0.56
1:C:24:ARG:HB2	1:C:26:ILE:HD12	1.87	0.56
1:A:10:ARG:HD3	1:A:62:ALA:O	2.04	0.56
1:D:24:ARG:NH2	1:D:57:GLU:OE1	2.37	0.56
1:C:44:ALA:O	1:C:46:LEU:N	2.38	0.55
1:C:100:SER:OG	1:C:124:THR:HG23	2.07	0.55
1:A:168:ASP:O	1:A:169:GLU:CB	2.55	0.55
1:B:167:GLN:NE2	1:B:169:GLU:O	2.40	0.55
1:B:137:TRP:CZ3	1:B:161:ILE:HG12	2.42	0.55
1:B:91:GLU:OE1	1:B:175:LEU:HD12	2.07	0.54
1:C:176:THR:CG2	1:C:180:VAL:CB	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD12	1:A:93:VAL:HG21	1.90	0.54
1:B:1:MET:HE2	1:B:43:PHE:CE1	2.40	0.54
1:B:97:ASP:HA	1:B:169:GLU:CB	2.38	0.54
1:C:176:THR:HG23	1:C:180:VAL:HB	1.90	0.54
1:A:151:VAL:HA	1:A:155:GLN:O	2.08	0.53
1:C:124:THR:HG22	1:C:126:ALA:H	1.73	0.53
1:B:168:ASP:O	1:B:169:GLU:CB	2.56	0.53
1:C:95:SER:HB3	1:D:85:LEU:HD12	1.90	0.53
1:A:109:SER:O	1:A:113:PHE:CD2	2.57	0.53
1:C:12:GLY:N	3:C:1189:PG4:H41	2.24	0.53
1:A:176:THR:H	3:A:1192:PG4:C1	2.22	0.52
1:A:89:LEU:CD1	1:A:93:VAL:HG21	2.40	0.52
1:C:173:HIS:HD2	5:C:2034:HOH:O	1.88	0.52
1:C:2:ARG:HB3	1:C:70:VAL:HG12	1.92	0.52
1:B:2:ARG:HA	1:B:41:LEU:O	2.10	0.51
1:B:1:MET:HE1	1:B:46:LEU:HB2	0.77	0.51
1:A:10:ARG:HG2	1:A:13:LEU:HD12	1.92	0.51
1:B:92:PRO:HB2	1:B:174:VAL:CG2	2.33	0.51
1:D:47:GLU:C	1:D:49:GLU:N	2.60	0.51
1:A:179:VAL:O	1:A:183:ARG:HG3	2.11	0.50
1:A:97:ASP:HA	1:A:169:GLU:CB	2.42	0.50
1:A:20:LEU:HD21	1:A:57:GLU:HG2	1.93	0.50
1:A:112:LEU:HD11	1:A:157:PHE:HZ	1.77	0.50
1:C:19:ASP:OD1	1:D:15:ARG:HD3	2.12	0.50
1:A:158:LEU:HB2	1:A:181:MET:HE1	1.94	0.49
1:A:176:THR:O	1:A:181:MET:HG3	2.13	0.49
1:C:78:GLU:OE1	1:C:78:GLU:CA	2.59	0.49
1:D:85:LEU:C	1:D:85:LEU:HD23	2.38	0.49
1:A:1:MET:HE3	1:A:43:PHE:HE1	1.78	0.49
1:B:165:TYR:HB3	1:B:168:ASP:OD2	2.12	0.49
1:A:180:VAL:HG11	3:A:1192:PG4:O2	2.13	0.48
1:B:34:ASP:HB3	1:B:38:ARG:HB2	1.93	0.48
1:C:33:ILE:CD1	1:D:28:LEU:HD23	2.41	0.48
1:B:115:GLN:HB2	1:B:120:LEU:HD13	1.96	0.48
1:D:97:ASP:HA	1:D:169:GLU:HB3	1.95	0.48
1:C:78:GLU:HG3	1:C:81:ALA:HB2	1.95	0.48
1:D:2:ARG:HD3	1:D:73:MET:HG2	1.95	0.48
1:B:147:ASN:HA	1:B:159:MET:O	2.14	0.48
1:C:51:PHE:CE2	1:C:55:MET:SD	3.06	0.48
1:D:31:ILE:HD11	1:D:33:ILE:CG1	2.40	0.48
1:C:10:ARG:HH11	1:C:10:ARG:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:VAL:HG23	1:D:170:ASN:HA	1.97	0.47
1:B:181:MET:O	1:B:185:THR:OG1	2.31	0.47
1:B:53:SER:O	1:B:57:GLU:HG3	2.15	0.47
1:C:1:MET:HG3	1:C:2:ARG:N	2.29	0.47
1:C:18:LEU:HD11	1:D:18:LEU:HD23	1.97	0.46
1:D:46:LEU:O	1:D:47:GLU:C	2.58	0.46
1:C:176:THR:HG22	1:C:180:VAL:HG21	1.92	0.46
1:A:15:ARG:HD3	1:B:19:ASP:OD1	2.16	0.46
1:B:27:ASP:HB3	1:B:44:ALA:HB3	1.98	0.46
1:C:78:GLU:HA	1:C:81:ALA:N	2.25	0.46
1:A:34:ASP:HA	1:A:35:PRO:HD2	1.69	0.46
1:C:115:GLN:HB2	1:C:120:LEU:HD13	1.97	0.46
1:D:146:HIS:NE2	1:D:148:GLU:OE1	2.34	0.45
1:D:71:PRO:HB2	1:D:72:TRP:CD1	2.52	0.45
1:A:85:LEU:C	1:A:85:LEU:HD12	2.42	0.45
1:D:31:ILE:HD11	1:D:33:ILE:CD1	2.47	0.45
1:D:97:ASP:HA	1:D:169:GLU:CB	2.47	0.45
1:B:1:MET:HB3	1:B:43:PHE:CE1	2.51	0.45
1:C:3:LEU:HD12	1:C:43:PHE:HZ	1.80	0.44
1:D:7:CYS:HB2	1:D:13:LEU:HD11	1.98	0.44
1:A:4:GLU:OE1	1:A:68:ARG:NH2	2.45	0.44
1:A:186:ILE:C	1:A:188:MET:H	2.25	0.44
1:C:17:LEU:O	1:C:21:LEU:HG	2.17	0.44
1:C:168:ASP:O	1:C:169:GLU:CB	2.64	0.44
1:A:146:HIS:HB3	1:A:161:ILE:CG2	2.47	0.44
1:B:4:GLU:OE2	1:B:38:ARG:HD3	2.18	0.44
1:A:92:PRO:HB2	1:A:174:VAL:HB	2.00	0.43
1:A:72:TRP:CE2	1:A:77:ARG:HG3	2.53	0.43
1:C:46:LEU:HD11	1:C:50:SER:HB2	2.01	0.43
1:C:76:GLU:HA	1:C:79:HIS:CE1	2.53	0.43
1:C:162:THR:O	1:C:170:ASN:HA	2.19	0.43
1:A:166:LEU:HB3	1:A:167:GLN:H	1.61	0.43
1:B:24:ARG:HB2	1:B:26:ILE:HD12	2.00	0.43
1:B:53:SER:O	1:B:57:GLU:CG	2.67	0.43
1:C:12:GLY:H	3:C:1189:PG4:H41	1.84	0.43
1:C:115:GLN:NE2	1:C:123:HIS:CD2	2.83	0.43
1:A:48:PHE:O	1:A:51:PHE:HB3	2.18	0.43
1:A:157:PHE:HB3	1:A:174:VAL:HG13	2.01	0.43
1:B:123:HIS:HA	1:B:127:GLN:NE2	2.33	0.43
1:A:112:LEU:HD11	1:A:157:PHE:CZ	2.53	0.42
1:A:10:ARG:HG3	1:A:13:LEU:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:HIS:NE2	1:B:89:LEU:CD2	2.79	0.42
1:A:1:MET:HG3	1:A:2:ARG:N	2.34	0.42
1:A:188:MET:O	1:A:189:GLY:C	2.63	0.42
1:A:175:LEU:HB2	1:A:181:MET:HE2	2.01	0.42
1:C:14:THR:HB	3:C:1189:PG4:C3	2.23	0.42
1:C:104:MET:HB2	1:C:104:MET:HE2	1.78	0.42
1:D:110:CYS:HB3	1:D:115:GLN:O	2.20	0.41
1:A:39:ILE:HD11	2:A:1191:AE3:H3C1	2.02	0.41
1:C:31:ILE:HA	1:C:40:TYR:O	2.20	0.41
1:D:137:TRP:CZ3	1:D:161:ILE:HG12	2.55	0.41
1:C:107:PRO:O	1:C:111:GLN:HG2	2.19	0.41
1:C:171:ASP:HB3	1:D:85:LEU:HG	2.01	0.41
1:A:146:HIS:HB3	1:A:161:ILE:HG22	2.03	0.41
1:B:47:GLU:H	1:B:47:GLU:HG3	1.65	0.41
1:C:176:THR:HG23	1:C:180:VAL:H	1.86	0.41
1:D:58:ILE:CG2	1:D:67:VAL:HG21	2.51	0.41
1:D:58:ILE:HG22	1:D:67:VAL:HG21	2.03	0.41
1:A:73:MET:O	1:A:74:PRO:C	2.62	0.40
1:C:96:VAL:HA	1:C:101:LYS:O	2.22	0.40
1:B:29:ARG:HD3	1:B:29:ARG:HA	1.88	0.40
1:B:86:LEU:CD2	1:B:104:MET:HE3	2.48	0.40
1:B:1:MET:HE3	1:B:43:PHE:HE1	1.82	0.40
1:B:165:TYR:CG	1:B:166:LEU:N	2.89	0.40
1:C:1:MET:HE2	1:C:1:MET:HB2	1.94	0.40
1:C:2:ARG:HA	1:C:41:LEU:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ILE:O	1:D:133:ASN:ND2[4_556]	1.87	0.33
1:B:59:ARG:NH1	1:C:49:GLU:OE1[1_554]	2.04	0.16

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	187/190 (98%)	170 (91%)	13 (7%)	4 (2%)	5	4
1	B	187/190 (98%)	178 (95%)	6 (3%)	3 (2%)	7	7
1	C	185/190 (97%)	169 (91%)	11 (6%)	5 (3%)	4	3
1	D	187/190 (98%)	175 (94%)	5 (3%)	7 (4%)	2	1
All	All	746/760 (98%)	692 (93%)	35 (5%)	19 (2%)	4	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	GLU
1	B	167	GLN
1	B	169	GLU
1	C	45	GLU
1	C	169	GLU
1	D	49	GLU
1	D	169	GLU
1	A	165	TYR
1	A	189	GLY
1	D	45	GLU
1	D	47	GLU
1	D	48	PHE
1	D	153	ASN
1	C	77	ARG
1	C	187	ARG
1	A	187	ARG
1	C	44	ALA
1	D	167	GLN
1	B	37	GLY

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	139/169 (82%)	117 (84%)	22 (16%)	2	2
1	B	155/169 (92%)	134 (86%)	21 (14%)	4	4
1	C	151/169 (89%)	135 (89%)	16 (11%)	6	8
1	D	144/169 (85%)	125 (87%)	19 (13%)	4	4
All	All	589/676 (87%)	511 (87%)	78 (13%)	4	4

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASP
1	A	10	ARG
1	A	11	LEU
1	A	31	ILE
1	A	46	LEU
1	A	67	VAL
1	A	70	VAL
1	A	80	LEU
1	A	82	LEU
1	A	85	LEU
1	A	109	SER
1	A	112	LEU
1	A	118	ASP
1	A	120	LEU
1	A	140	SER
1	A	151	VAL
1	A	158	LEU
1	A	171	ASP
1	A	172	GLN
1	A	180	VAL
1	A	185	THR
1	B	1	MET
1	B	9	ASP
1	B	10	ARG
1	B	17	LEU
1	B	46	LEU
1	B	47	GLU
1	B	48	PHE
1	B	57	GLU
1	B	67	VAL
1	B	101	LYS
1	B	104	MET

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Mol	Chain	Res	Type
1	B	118	ASP
1	B	119	ARG
1	B	120	LEU
1	B	135	LEU
1	B	138	LEU
1	B	140	SER
1	B	156	ASN
1	B	166	LEU
1	B	175	LEU
1	B	185	THR
1	C	1	MET
1	C	10	ARG
1	C	17	LEU
1	C	26	ILE
1	C	43	PHE
1	C	67	VAL
1	C	69	THR
1	C	70	VAL
1	C	76	GLU
1	C	78	GLU
1	C	83	SER
1	C	87	GLU
1	C	104	MET
1	C	138	LEU
1	C	151	VAL
1	C	175	LEU
1	D	13	LEU
1	D	18	LEU
1	D	20	LEU
1	D	31	ILE
1	D	38	ARG
1	D	52	SER
1	D	70	VAL
1	D	80	LEU
1	D	82	LEU
1	D	85	LEU
1	D	94	LEU
1	D	104	MET
1	D	111	GLN
1	D	120	LEU
1	D	138	LEU
1	D	139	GLU

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Mol	Chain	Res	Type
1	D	162	THR
1	D	168	ASP
1	D	185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	147	ASN
1	A	172	GLN
1	B	42	ASN
1	B	115	GLN
1	B	122	ASN
1	B	123	HIS
1	B	130	ASN
1	B	147	ASN
1	B	149	HIS
1	B	156	ASN
1	C	79	HIS
1	C	111	GLN
1	C	115	GLN
1	C	133	ASN
1	C	143	GLN
1	C	153	ASN
1	C	173	HIS
1	D	111	GLN
1	D	167	GLN
1	D	173	HIS

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

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	$\# Z > 2$
3	PG4	C	1189	-	11,11,12	0.77	0	10,10,11	0.43	0
2	AE3	A	1191	-	8,8,8	0.74	0	7,7,7	0.52	0
4	SO4	B	1191	-	4,4,4	0.37	0	6,6,6	0.65	0
3	PG4	A	1192	-	11,11,12	0.55	0	10,10,11	0.40	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
3	PG4	C	1189	-	-	7/9/9/10	-
2	AE3	A	1191	-	-	6/6/6/6	-
3	PG4	A	1192	-	-	4/9/9/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1192	PG4	O2-C3-C4-O3
2	A	1191	AE3	O2-C3-C4-O3
2	A	1191	AE3	O3-C5-C6-O4
3	A	1192	PG4	O4-C7-C8-O5
3	A	1192	PG4	O3-C5-C6-O4
3	C	1189	PG4	O2-C3-C4-O3
3	C	1189	PG4	C1-C2-O2-C3
3	C	1189	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	A	1191	AE3	C6-C5-O3-C4
3	C	1189	PG4	O3-C5-C6-O4
2	A	1191	AE3	C4-C3-O2-C2
3	A	1192	PG4	C4-C3-O2-C2
2	A	1191	AE3	C3-C4-O3-C5
3	C	1189	PG4	C8-C7-O4-C6
3	C	1189	PG4	C4-C3-O2-C2
3	C	1189	PG4	C5-C6-O4-C7
2	A	1191	AE3	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1189	PG4	9	0
2	A	1191	AE3	1	0
3	A	1192	PG4	5	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	189/190 (99%)	1.22	30 (15%) 5 5	24, 39, 50, 55	0
1	B	189/190 (99%)	1.10	29 (15%) 5 6	23, 43, 51, 57	0
1	C	187/190 (98%)	1.27	37 (19%) 3 3	30, 42, 54, 66	0
1	D	189/190 (99%)	1.49	50 (26%) 1 2	34, 43, 54, 57	0
All	All	754/760 (99%)	1.27	146 (19%) 3 3	23, 42, 52, 66	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	9.3
1	A	166	LEU	8.4
1	D	48	PHE	6.1
1	D	189	GLY	5.8
1	D	50	SER	5.2
1	D	46	LEU	5.1
1	A	154	GLY	4.9
1	D	190	ARG	4.8
1	A	137	TRP	4.7
1	B	166	LEU	4.6
1	D	118	ASP	4.6
1	C	79	HIS	4.5
1	B	165	TYR	3.9
1	A	165	TYR	3.9
1	D	178	ALA	3.8
1	A	167	GLN	3.8
1	C	171	ASP	3.7
1	B	167	GLN	3.7
1	B	36	ILE	3.6
1	B	189	GLY	3.6
1	A	180	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	36	ILE	3.5
1	D	45	GLU	3.5
1	A	142	PRO	3.4
1	D	115	GLN	3.4
1	D	186	ILE	3.3
1	D	79	HIS	3.3
1	B	79	HIS	3.3
1	C	180	VAL	3.3
1	B	171	ASP	3.2
1	D	158	LEU	3.2
1	C	75	SER	3.2
1	B	164	VAL	3.2
1	D	180	VAL	3.2
1	A	85	LEU	3.2
1	A	35	PRO	3.2
1	C	166	LEU	3.2
1	D	51	PHE	3.0
1	A	190	ARG	3.0
1	D	119	ARG	3.0
1	D	44	ALA	3.0
1	B	180	VAL	2.9
1	D	47	GLU	2.9
1	C	168	ASP	2.9
1	C	119	ARG	2.9
1	A	47	GLU	2.9
1	C	71	PRO	2.9
1	B	190	ARG	2.8
1	A	80	LEU	2.8
1	C	140	SER	2.8
1	C	78	GLU	2.8
1	D	176	THR	2.8
1	D	64	VAL	2.8
1	D	174	VAL	2.8
1	D	182	LEU	2.7
1	B	48	PHE	2.7
1	A	79	HIS	2.7
1	D	173	HIS	2.7
1	A	189	GLY	2.7
1	A	102	VAL	2.7
1	D	122	ASN	2.7
1	C	81	ALA	2.7
1	D	22	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	178	ALA	2.6
1	D	84	ALA	2.6
1	B	23	LEU	2.6
1	A	130	ASN	2.6
1	B	114	GLY	2.6
1	B	176	THR	2.6
1	C	84	ALA	2.6
1	A	182	LEU	2.6
1	D	80	LEU	2.6
1	A	141	GLU	2.5
1	C	76	GLU	2.5
1	A	187	ARG	2.5
1	B	13	LEU	2.5
1	C	142	PRO	2.5
1	A	126	ALA	2.5
1	D	63	GLY	2.5
1	C	172	GLN	2.5
1	B	174	VAL	2.5
1	C	80	LEU	2.5
1	A	168	ASP	2.5
1	B	12	GLY	2.5
1	D	120	LEU	2.4
1	A	81	ALA	2.4
1	D	49	GLU	2.4
1	D	83	SER	2.4
1	C	13	LEU	2.4
1	D	114	GLY	2.4
1	A	110	CYS	2.4
1	B	119	ARG	2.4
1	B	47	GLU	2.4
1	D	90	PRO	2.4
1	D	77	ARG	2.4
1	D	78	GLU	2.4
1	C	34	ASP	2.3
1	C	165	TYR	2.3
1	C	37	GLY	2.3
1	A	108	ALA	2.3
1	A	164	VAL	2.3
1	C	35	PRO	2.3
1	C	96	VAL	2.3
1	B	53	SER	2.2
1	A	135	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	168	ASP	2.2
1	C	45	GLU	2.2
1	A	83	SER	2.2
1	D	145	SER	2.2
1	A	36	ILE	2.2
1	C	161	ILE	2.2
1	B	1	MET	2.2
1	A	151	VAL	2.2
1	C	154	GLY	2.2
1	D	12	GLY	2.2
1	A	88	ALA	2.2
1	B	140	SER	2.2
1	D	81	ALA	2.2
1	D	20	LEU	2.1
1	D	39	ILE	2.1
1	C	174	VAL	2.1
1	C	83	SER	2.1
1	C	108	ALA	2.1
1	D	162	THR	2.1
1	C	77	ARG	2.1
1	B	50	SER	2.1
1	C	55	MET	2.1
1	C	182	LEU	2.1
1	D	31	ILE	2.1
1	D	96	VAL	2.1
1	D	179	VAL	2.1
1	C	72	TRP	2.1
1	D	183	ARG	2.1
1	C	124	THR	2.1
1	D	99	LYS	2.1
1	D	188	MET	2.1
1	B	33	ILE	2.1
1	B	118	ASP	2.1
1	B	173	HIS	2.1
1	B	178	ALA	2.0
1	B	172	GLN	2.0
1	B	168	ASP	2.0
1	C	122	ASN	2.0
1	D	117	LEU	2.0
1	C	56	ALA	2.0
1	D	82	LEU	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($\text{\AA}^2$)	Q<0.9
3	PG4	A	1192	12/13	0.71	0.16	52,62,70,71	0
3	PG4	C	1189	12/13	0.71	0.17	31,44,60,60	0
2	AE3	A	1191	9/9	0.87	0.12	40,52,53,54	0
4	SO4	B	1191	5/5	0.95	0.17	33,39,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.