



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:57 AM UTC

PDB ID : 6AH7 / pdb_00006ah7
Title : D45W/H226G mutant of marine bacterial prolidase
Authors : Jian, Y.; Yunzhu, X.; Lijuan, L.
Deposited on : 2018-08-17
Resolution : 2.38 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

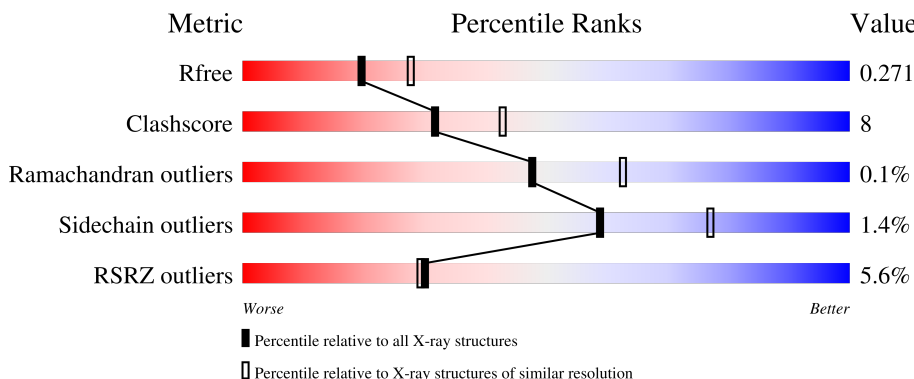
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	448	
1	B	448	
1	C	448	
1	D	448	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14924 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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	1	0
			3573	2297	608	654	14			
1	B	439	Total	C	N	O	S	0	4	0
			3604	2315	618	657	14			
1	C	439	Total	C	N	O	S	0	2	0
			3584	2303	612	655	14			
1	D	439	Total	C	N	O	S	0	2	0
			3584	2303	612	655	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
A	226	GLY	HIS	engineered mutation	UNP A0A1I7CHQ2
A	441	LEU	-	expression tag	UNP A0A1I7CHQ2
A	442	ASP	-	expression tag	UNP A0A1I7CHQ2
A	443	HIS	-	expression tag	UNP A0A1I7CHQ2
A	444	HIS	-	expression tag	UNP A0A1I7CHQ2
A	445	HIS	-	expression tag	UNP A0A1I7CHQ2
A	446	HIS	-	expression tag	UNP A0A1I7CHQ2
A	447	HIS	-	expression tag	UNP A0A1I7CHQ2
A	448	HIS	-	expression tag	UNP A0A1I7CHQ2
B	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
B	226	GLY	HIS	engineered mutation	UNP A0A1I7CHQ2
B	441	LEU	-	expression tag	UNP A0A1I7CHQ2
B	442	ASP	-	expression tag	UNP A0A1I7CHQ2
B	443	HIS	-	expression tag	UNP A0A1I7CHQ2
B	444	HIS	-	expression tag	UNP A0A1I7CHQ2
B	445	HIS	-	expression tag	UNP A0A1I7CHQ2
B	446	HIS	-	expression tag	UNP A0A1I7CHQ2
B	447	HIS	-	expression tag	UNP A0A1I7CHQ2
B	448	HIS	-	expression tag	UNP A0A1I7CHQ2
C	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	226	GLY	HIS	engineered mutation	UNP A0A1I7CHQ2
C	441	LEU	-	expression tag	UNP A0A1I7CHQ2
C	442	ASP	-	expression tag	UNP A0A1I7CHQ2
C	443	HIS	-	expression tag	UNP A0A1I7CHQ2
C	444	HIS	-	expression tag	UNP A0A1I7CHQ2
C	445	HIS	-	expression tag	UNP A0A1I7CHQ2
C	446	HIS	-	expression tag	UNP A0A1I7CHQ2
C	447	HIS	-	expression tag	UNP A0A1I7CHQ2
C	448	HIS	-	expression tag	UNP A0A1I7CHQ2
D	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
D	226	GLY	HIS	engineered mutation	UNP A0A1I7CHQ2
D	441	LEU	-	expression tag	UNP A0A1I7CHQ2
D	442	ASP	-	expression tag	UNP A0A1I7CHQ2
D	443	HIS	-	expression tag	UNP A0A1I7CHQ2
D	444	HIS	-	expression tag	UNP A0A1I7CHQ2
D	445	HIS	-	expression tag	UNP A0A1I7CHQ2
D	446	HIS	-	expression tag	UNP A0A1I7CHQ2
D	447	HIS	-	expression tag	UNP A0A1I7CHQ2
D	448	HIS	-	expression tag	UNP A0A1I7CHQ2

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

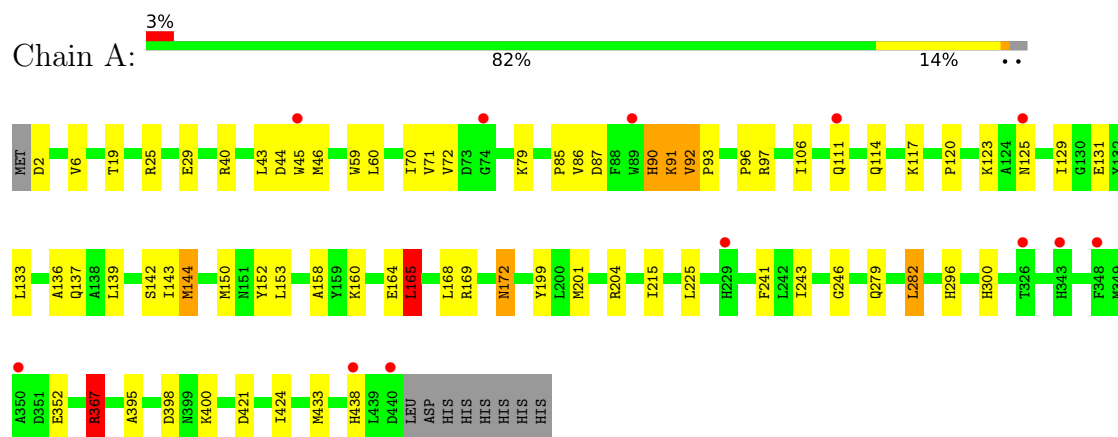
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	160	Total	O	0	0
			160	160		
5	C	110	Total	O	0	0
			110	110		
5	D	139	Total	O	0	0
			139	139		

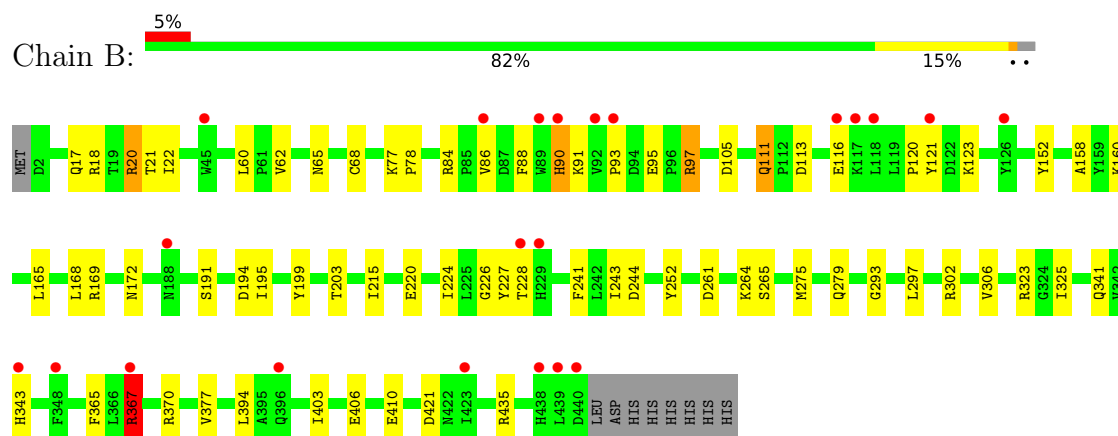
3 Residue-property plots [i](#)

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.

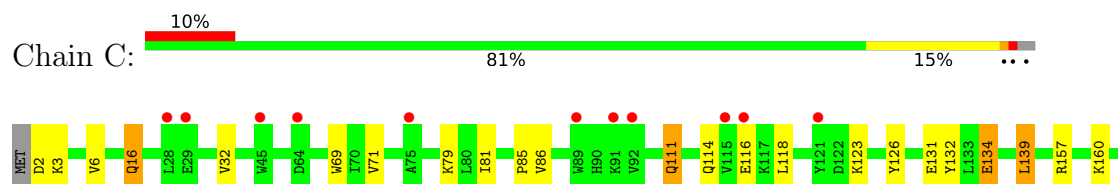
• Molecule 1: Xaa-Pro dipeptidase

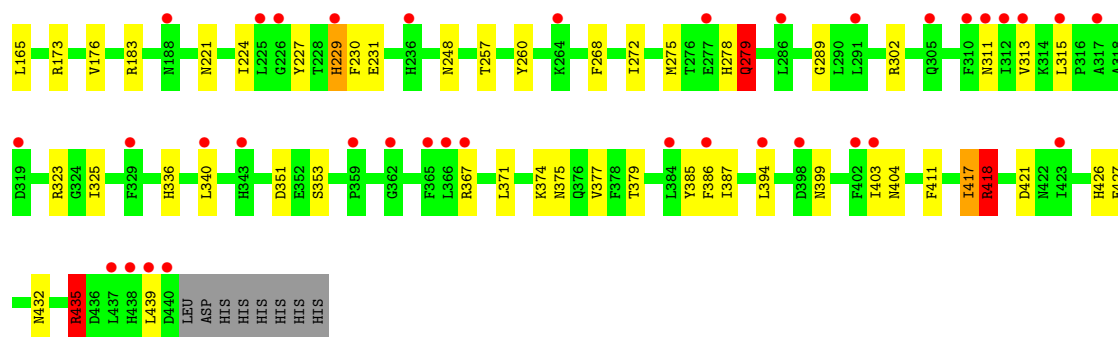


• Molecule 1: Xaa-Pro dipeptidase

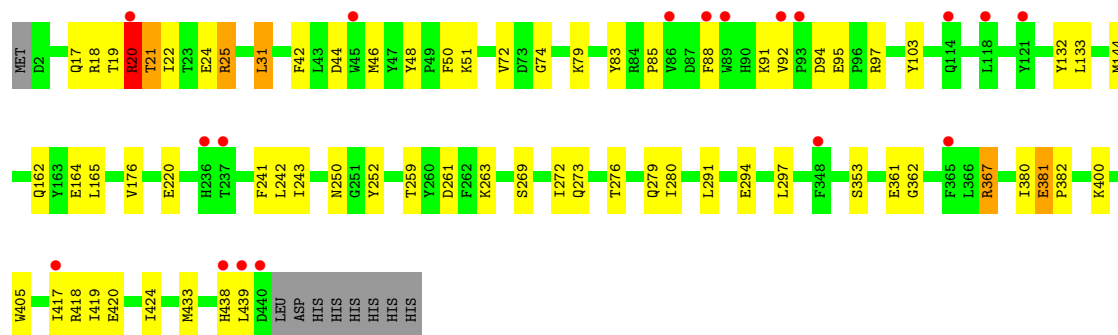
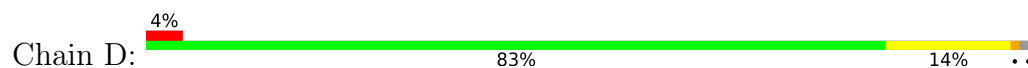


• Molecule 1: Xaa-Pro dipeptidase





● Molecule 1: Xaa-Pro dipeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	183.63Å 183.63Å 371.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.29 – 2.38 67.29 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.8 (67.29-2.38) 94.7 (67.29-2.38)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.233 , 0.269 0.237 , 0.271	Depositor DCC
R_{free} test set	4428 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14924	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% 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, NA, MN

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	0.63	9/3677 (0.2%)	0.65	6/4993 (0.1%)
1	B	0.44	3/3710 (0.1%)	0.57	4/5037 (0.1%)
1	C	0.46	5/3688 (0.1%)	0.54	5/5007 (0.1%)
1	D	0.52	1/3688 (0.0%)	0.63	5/5007 (0.1%)
All	All	0.52	18/14763 (0.1%)	0.60	20/20044 (0.1%)

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	3
1	B	0	4
1	C	0	2
1	D	0	5
All	All	0	14

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	382	PRO	C-O	-7.81	1.14	1.23
1	C	85	PRO	C-O	-6.55	1.16	1.23
1	A	164	GLU	C-O	-6.35	1.16	1.24
1	A	165	LEU	C-O	-6.29	1.16	1.24
1	A	90	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	85	PRO	C-O	-5.94	1.17	1.23
1	A	172	ASN	C-O	-5.53	1.17	1.24
1	A	96	PRO	C-O	-5.46	1.16	1.24
1	B	21	THR	C-O	-5.39	1.17	1.24
1	C	229	HIS	ND1-CE1	5.33	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ILE	C-O	-5.29	1.18	1.24
1	A	296	HIS	ND1-CE1	5.25	1.37	1.32
1	A	300	HIS	ND1-CE1	5.21	1.37	1.32
1	B	20	ARG	C-O	-5.15	1.18	1.24
1	C	111	GLN	CD-OE1	5.11	1.33	1.23
1	C	279	GLN	C-O	-5.11	1.18	1.24
1	C	16	GLN	CD-OE1	5.03	1.33	1.23
1	B	111	GLN	CD-OE1	5.02	1.33	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	HIS	CB-CG-CD2	-7.19	121.86	131.20
1	D	21	THR	N-CA-CB	6.93	122.20	110.49
1	A	296	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	A	300	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	C	229	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	A	90	HIS	CB-CG-ND1	6.30	132.15	122.70
1	D	20	ARG	CA-C-O	-6.02	113.45	120.62
1	D	20	ARG	N-CA-C	-5.98	100.54	109.15
1	B	367	ARG	CB-CA-C	5.77	119.79	109.29
1	A	296	HIS	CB-CG-ND1	5.67	131.21	122.70
1	A	300	HIS	CB-CG-ND1	5.61	131.11	122.70
1	C	229	HIS	CB-CG-ND1	5.58	131.06	122.70
1	C	132	TYR	CB-CA-C	5.45	120.30	112.12
1	B	367	ARG	CB-CG-CD	5.43	123.80	111.30
1	B	121	TYR	CA-C-N	-5.18	116.10	122.84
1	B	121	TYR	C-N-CA	-5.18	116.10	122.84
1	C	435	ARG	CB-CA-C	5.14	120.53	110.67
1	D	380	ILE	CA-C-N	5.05	134.13	121.80
1	D	380	ILE	C-N-CA	5.05	134.13	121.80
1	C	139	LEU	N-CA-C	-5.03	106.65	112.89

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ARG	Sidechain
1	A	367	ARG	Sidechain
1	A	97	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	367	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	90[B]	HIS	Mainchain
1	B	97	ARG	Sidechain
1	C	367	ARG	Sidechain
1	C	418	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	20	ARG	Sidechain
1	D	25	ARG	Sidechain
1	D	367	ARG	Sidechain
1	D	418	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3573	0	3429	56	0
1	B	3604	0	3453	61	0
1	C	3584	0	3441	61	0
1	D	3584	0	3441	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	1	0
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	156	0	0	7	0
5	B	160	0	0	5	1
5	C	110	0	0	7	2
5	D	139	0	0	10	1
All	All	14924	0	13764	227	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 8.

All (227) 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:381:GLU:CD	1:D:420:GLU:OE2	1.81	1.23
1:D:381:GLU:HG3	1:D:420:GLU:HG3	1.27	1.15
1:D:381:GLU:HG3	1:D:420:GLU:CG	1.78	1.12
1:D:261:ASP:OD1	1:D:263:LYS:O	1.79	1.00
1:A:424:ILE:HD11	1:A:433:MET:HE3	1.50	0.92
1:D:381:GLU:HG3	1:D:420:GLU:CD	1.94	0.92
1:A:19:THR:HG21	1:A:72:VAL:HG12	1.52	0.88
1:D:424:ILE:HD11	1:D:433:MET:HE3	1.60	0.84
1:D:272:ILE:HG12	1:D:417:ILE:HD12	1.58	0.83
1:D:381:GLU:CG	1:D:420:GLU:CD	2.52	0.82
1:D:85:PRO:O	1:D:92:VAL:CG1	2.30	0.79
1:D:381:GLU:OE1	5:D:601:HOH:O	1.99	0.78
1:D:17:GLN:O	1:D:20:ARG:O	2.01	0.77
1:C:71:VAL:HG12	1:C:79:LYS:HB2	1.67	0.75
1:D:85:PRO:O	1:D:92:VAL:HG11	1.87	0.75
1:D:381:GLU:OE2	1:D:420:GLU:OE2	2.03	0.75
1:D:20:ARG:NE	1:D:24:GLU:OE1	2.19	0.73
1:A:133:LEU:HB3	1:A:144:MET:HE2	1.70	0.73
1:C:32:VAL:HG22	1:C:71:VAL:HG23	1.71	0.73
1:B:394:LEU:HD21	1:B:403:ILE:HD11	1.70	0.72
1:A:131:GLU:OE1	5:A:601:HOH:O	2.06	0.72
1:D:94:ASP:HB3	1:D:97:ARG:NH2	2.03	0.72
1:D:31:LEU:HD12	1:D:72:VAL:HG23	1.70	0.72
1:B:22:ILE:HD13	1:B:152:TYR:CG	2.26	0.70
1:D:94:ASP:HB3	1:D:97:ARG:HH22	1.53	0.70
1:D:44:ASP:OD2	5:D:602:HOH:O	2.09	0.69
1:D:381:GLU:CD	1:D:420:GLU:CD	2.61	0.69
1:A:106:ILE:O	5:A:602:HOH:O	2.09	0.69
1:A:398:ASP:OD2	5:A:603:HOH:O	2.11	0.68
1:D:19:THR:HG23	1:D:31:LEU:HD11	1.73	0.68
1:B:168:LEU:HD23	1:B:252:TYR:HB3	1.75	0.68
1:C:2:ASP:OD1	1:C:3:LYS:N	2.27	0.68
1:C:248:ASN:OD1	5:C:601:HOH:O	2.12	0.67
1:C:157:ARG:CZ	1:C:340:LEU:HD12	2.25	0.67
1:A:438:HIS:NE2	1:D:438:HIS:NE2	2.43	0.67
1:C:157:ARG:NE	1:C:340:LEU:HD12	2.10	0.66
1:B:60:LEU:HD13	1:B:62:VAL:CG2	2.25	0.66
1:C:426:HIS:O	5:C:602:HOH:O	2.12	0.66
1:D:48:TYR:OH	5:D:603:HOH:O	2.09	0.65
1:C:71:VAL:CG1	1:C:79:LYS:HD2	2.27	0.65
1:B:265:SER:O	5:B:601:HOH:O	2.13	0.65
1:D:250:ASN:OD1	5:D:604:HOH:O	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:TYR:O	5:D:605:HOH:O	2.15	0.64
1:C:126:TYR:O	5:C:603:HOH:O	2.14	0.64
1:D:420:GLU:OE2	2:D:501:MN:MN	1.55	0.64
1:C:311:ASN:OD1	1:C:404:ASN:ND2	2.30	0.64
1:C:16:GLN:NE2	5:C:606:HOH:O	2.30	0.64
1:D:95:GLU:O	1:D:97:ARG:NH1	2.31	0.64
1:D:85:PRO:O	1:D:92:VAL:HG12	1.98	0.63
1:A:19:THR:HG21	1:A:72:VAL:CG1	2.26	0.63
1:A:87:ASP:HB2	1:A:90:HIS:ND1	2.14	0.62
1:B:60:LEU:HD13	1:B:62:VAL:HG23	1.81	0.62
1:C:221:ASN:HA	1:C:224:ILE:HD12	1.81	0.62
1:A:111:GLN:HB2	1:A:114:GLN:NE2	2.14	0.62
1:A:367:ARG:H	1:A:367:ARG:CD	2.11	0.62
1:A:86:VAL:HG23	1:A:86:VAL:O	1.99	0.62
1:B:90[B]:HIS:ND1	1:B:91:LYS:N	2.45	0.62
1:B:199:TYR:O	1:B:203:THR:HG23	1.99	0.62
1:B:120:PRO:O	1:B:123:LYS:NZ	2.33	0.61
1:B:394:LEU:HD23	1:B:403:ILE:HD13	1.82	0.61
1:D:361:GLU:HG2	1:D:362:GLY:N	2.16	0.61
1:B:111:GLN:NE2	1:B:113:ASP:OD1	2.28	0.61
1:D:269:SER:O	1:D:273:GLN:HG2	2.00	0.61
1:A:91:LYS:HE2	1:B:228:THR:H	1.65	0.61
1:B:394:LEU:CD2	1:B:403:ILE:HD11	2.31	0.61
1:A:44:ASP:OD2	5:A:604:HOH:O	2.16	0.60
1:C:111:GLN:OE1	1:C:114:GLN:OE1	2.20	0.60
1:B:394:LEU:CD2	1:B:403:ILE:CD1	2.80	0.59
1:C:421:ASP:OD2	1:C:435:ARG:NE	2.35	0.59
1:B:86:VAL:HG22	1:B:86:VAL:O	2.02	0.59
1:B:323:ARG:HB2	1:B:325:ILE:HD12	1.86	0.58
1:A:92:VAL:HG12	1:A:92:VAL:O	2.04	0.58
1:C:435:ARG:HG2	1:C:435:ARG:HH21	1.67	0.58
1:C:375:ASN:OD1	5:C:604:HOH:O	2.18	0.57
1:B:111:GLN:HE21	1:B:113:ASP:CG	2.12	0.57
1:B:95:GLU:O	1:B:97:ARG:HG3	2.04	0.57
1:C:394:LEU:HD11	1:C:403:ILE:HD11	1.85	0.57
1:C:435:ARG:HH21	1:C:435:ARG:CG	2.16	0.57
1:A:29:GLU:HG3	1:A:125:ASN:HB2	1.87	0.56
1:D:381:GLU:CG	1:D:420:GLU:OE2	2.51	0.56
1:A:367:ARG:NH1	5:A:607:HOH:O	2.39	0.56
1:D:31:LEU:HD12	1:D:72:VAL:CG2	2.35	0.56
1:A:2:ASP:O	1:A:6:VAL:HG23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MET:HE2	1:B:306:VAL:HG21	1.88	0.56
1:C:257:THR:HG21	1:C:418:ARG:HG2	1.88	0.56
1:D:279:GLN:HG3	1:D:419:ILE:HB	1.88	0.55
1:B:158:ALA:HA	5:B:634:HOH:O	2.07	0.55
1:D:20:ARG:HB2	1:D:74:GLY:HA3	1.88	0.54
1:B:22:ILE:HD13	1:B:152:TYR:CB	2.37	0.54
1:B:160:LYS:HD2	5:B:647:HOH:O	2.08	0.54
1:C:374:LYS:HD3	1:C:427:GLU:HB2	1.90	0.54
1:B:172:ASN:ND2	5:B:606:HOH:O	2.39	0.54
1:A:136:ALA:HB3	1:A:144:MET:HE3	1.90	0.54
1:C:313:VAL:HG12	1:C:315:LEU:HB2	1.90	0.53
1:D:291:LEU:HB3	5:D:625:HOH:O	2.09	0.53
1:D:294:GLU:HA	1:D:297:LEU:HD12	1.90	0.53
1:D:276:THR:O	1:D:280:ILE:HG13	2.08	0.53
1:D:164:GLU:HG2	1:D:252:TYR:OH	2.09	0.53
1:A:137:GLN:HG3	1:A:144:MET:HE1	1.90	0.53
1:A:59:TRP:CZ2	1:A:72:VAL:HG11	2.43	0.53
1:D:164:GLU:HG2	1:D:252:TYR:CZ	2.44	0.52
1:A:43:LEU:O	1:B:341:GLN:NE2	2.41	0.52
1:A:367:ARG:H	1:A:367:ARG:HD2	1.73	0.52
1:C:71:VAL:HG11	1:C:79:LYS:HD2	1.91	0.52
1:D:132:TYR:OH	5:D:606:HOH:O	2.17	0.52
1:A:60:LEU:HD21	1:A:70:ILE:HD11	1.91	0.52
1:A:152:TYR:HD2	1:A:153:LEU:HD12	1.74	0.51
1:C:229:HIS:NE2	1:C:231:GLU:OE1	2.37	0.51
1:C:289:GLY:C	1:C:371:LEU:HD11	2.35	0.51
1:D:51:LYS:HA	5:D:614:HOH:O	2.09	0.51
1:D:400:LYS:HG2	1:D:405:TRP:HE1	1.75	0.51
1:C:116:GLU:C	1:C:118:LEU:H	2.18	0.51
1:C:229:HIS:ND1	1:C:230:PHE:N	2.58	0.51
1:A:133:LEU:HB3	1:A:144:MET:CE	2.40	0.51
1:C:116:GLU:OE2	1:C:123:LYS:NZ	2.37	0.51
1:D:133:LEU:HB3	1:D:144:MET:HE3	1.94	0.50
1:A:395:ALA:O	1:A:400:LYS:HE2	2.12	0.50
1:B:77:LYS:HG3	1:B:78:PRO:HD2	1.94	0.50
1:B:394:LEU:HD21	1:B:403:ILE:CD1	2.40	0.50
1:C:2:ASP:O	1:C:6:VAL:HG13	2.11	0.50
1:B:60:LEU:CD1	1:B:62:VAL:HB	2.42	0.50
1:B:191:SER:OG	1:B:194:ASP:OD2	2.29	0.50
1:B:261:ASP:OD2	1:B:264:LYS:N	2.46	0.49
1:C:173:ARG:HB2	1:C:173:ARG:NH2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HD12	1:A:150:MET:HE3	1.94	0.49
1:C:221:ASN:OD1	1:D:91:LYS:NZ	2.35	0.48
1:C:435:ARG:CG	1:C:435:ARG:NH2	2.73	0.48
1:A:91:LYS:HE3	1:B:227:TYR:HA	1.95	0.48
1:C:323:ARG:HD2	1:C:399:ASN:OD1	2.13	0.48
1:C:385:TYR:OH	1:C:418:ARG:HD3	2.13	0.48
1:C:69:TRP:HB2	1:C:81:ILE:HB	1.96	0.48
1:C:131:GLU:HB2	1:D:42:PHE:CD1	2.49	0.48
1:C:176:VAL:HG13	1:C:439:LEU:HD13	1.94	0.48
1:A:120:PRO:O	1:A:123:LYS:HE3	2.13	0.48
1:C:279:GLN:HE21	1:C:279:GLN:HB2	1.49	0.48
1:A:6:VAL:HG21	1:D:162:GLN:HG3	1.95	0.48
1:B:215:ILE:HB	1:B:244:ASP:HB3	1.96	0.48
1:C:323:ARG:HB2	1:C:325:ILE:HD13	1.96	0.47
1:D:241:PHE:CZ	1:D:243:ILE:HB	2.49	0.47
1:A:123:LYS:NZ	1:A:139:LEU:O	2.36	0.47
1:A:215:ILE:HA	5:A:640:HOH:O	2.12	0.47
1:D:83:TYR:CZ	1:D:85:PRO:HG3	2.49	0.47
1:B:394:LEU:HD23	1:B:403:ILE:CD1	2.45	0.47
1:C:173:ARG:HB2	1:C:173:ARG:HH21	1.80	0.47
1:A:160:LYS:HB2	1:A:165:LEU:HD13	1.95	0.47
1:D:242:LEU:HD23	1:D:259:THR:OG1	2.15	0.46
1:C:268:PHE:CE2	1:C:272:ILE:HD11	2.50	0.46
1:D:361:GLU:HG2	1:D:362:GLY:H	1.79	0.46
1:A:168:LEU:CB	1:A:433:MET:HE1	2.45	0.46
1:B:88:PHE:CD1	1:B:88:PHE:C	2.94	0.46
1:C:351:ASP:OD1	1:C:353:SER:OG	2.31	0.46
1:C:387:ILE:HG21	1:D:88:PHE:HB2	1.96	0.46
1:D:381:GLU:OE1	1:D:420:GLU:OE2	2.28	0.46
1:C:3:LYS:O	1:C:6:VAL:HG22	2.16	0.46
1:B:168:LEU:HD12	1:B:377:VAL:HG21	1.98	0.46
1:D:176:VAL:HG13	1:D:439:LEU:HB2	1.99	0.45
1:C:432:ASN:CG	1:C:435:ARG:HB2	2.41	0.45
1:B:17:GLN:CD	1:B:20:ARG:HH21	2.25	0.45
1:C:134:GLU:CD	1:C:134:GLU:H	2.25	0.45
1:A:91:LYS:O	1:A:93:PRO:HD3	2.17	0.45
1:A:201:MET:HE3	1:A:201:MET:HB3	1.83	0.45
1:C:160:LYS:HG3	1:C:377:VAL:HG23	1.99	0.45
1:D:220:GLU:CD	1:D:220:GLU:H	2.23	0.45
1:B:84:ARG:NH1	1:B:84:ARG:HG2	2.31	0.45
1:B:302:ARG:O	1:B:306:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:CD2	1:B:403:ILE:HD13	2.45	0.45
1:C:123:LYS:O	5:C:603:HOH:O	2.20	0.45
1:D:50:PHE:HA	5:D:624:HOH:O	2.17	0.45
1:A:133:LEU:O	1:A:144:MET:HE1	2.17	0.45
1:B:279:GLN:HE22	1:B:421:ASP:CG	2.25	0.45
1:C:160:LYS:HB2	1:C:165:LEU:CD1	2.47	0.44
1:B:220:GLU:CD	1:B:220:GLU:H	2.25	0.44
1:B:406:GLU:O	1:B:410:GLU:HG3	2.17	0.44
1:C:116:GLU:HG2	1:C:139:LEU:HD22	1.99	0.44
1:C:183:ARG:HG3	1:C:260:TYR:CE2	2.52	0.44
1:C:2:ASP:CG	1:C:3:LYS:N	2.70	0.44
1:D:22:ILE:HD12	1:D:22:ILE:HA	1.85	0.44
1:B:195:ILE:HG21	1:B:241:PHE:CZ	2.53	0.44
1:C:116:GLU:C	1:C:118:LEU:N	2.74	0.44
1:C:275:MET:HG2	1:C:417:ILE:HD11	2.00	0.44
1:A:225:LEU:HD12	1:B:88:PHE:HE1	1.83	0.44
1:C:386:PHE:CE2	1:C:411:PHE:HB3	2.53	0.44
1:A:45:TRP:CZ3	1:B:343[B]:HIS:HB3	2.53	0.43
1:A:133:LEU:O	1:A:144:MET:CE	2.66	0.43
1:C:353:SER:HA	5:C:607:HOH:O	2.18	0.43
1:B:84:ARG:HG3	1:B:93:PRO:HG2	2.00	0.43
1:B:84:ARG:CG	1:B:84:ARG:HH11	2.31	0.43
1:C:227:TYR:CZ	1:C:229:HIS:HB3	2.53	0.43
1:B:60:LEU:HD13	1:B:62:VAL:HB	2.01	0.43
1:A:215:ILE:O	1:A:243:ILE:HA	2.18	0.43
1:C:403:ILE:N	1:C:403:ILE:HD12	2.34	0.43
1:D:353:SER:O	5:D:609:HOH:O	2.22	0.43
1:C:336:HIS:CE1	1:C:379:THR:HG21	2.54	0.42
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.89	0.42
1:A:158:ALA:HA	5:A:626:HOH:O	2.20	0.42
1:A:241:PHE:CZ	1:A:243:ILE:HB	2.54	0.42
1:B:279:GLN:OE1	1:B:435:ARG:NH1	2.49	0.42
1:A:40:ARG:NH2	3:A:503:SO4:O1	2.53	0.42
1:A:279:GLN:HE22	1:A:421:ASP:CG	2.28	0.42
1:A:199:TYR:OH	1:A:246:GLY:O	2.35	0.42
1:B:65:ASN:ND2	1:B:68:CYS:SG	2.93	0.42
1:B:226:GLY:O	1:B:228:THR:HG23	2.20	0.42
1:B:323:ARG:HB2	1:B:325:ILE:CD1	2.48	0.42
1:A:91:LYS:H	1:A:91:LYS:HG2	1.29	0.42
1:B:168:LEU:CD2	1:B:252:TYR:HB3	2.47	0.41
1:B:293:GLY:O	1:B:297:LEU:HD13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.86	0.41
1:A:165:LEU:HG	1:A:424:ILE:HD13	2.01	0.41
1:B:77:LYS:HE3	1:B:105:ASP:OD2	2.21	0.41
1:B:165:LEU:O	1:B:169:ARG:HG3	2.20	0.41
1:C:278:HIS:ND1	1:C:302:ARG:HD3	2.35	0.41
1:A:133:LEU:CB	1:A:144:MET:HE2	2.46	0.41
1:A:117:LYS:HD3	1:A:117:LYS:HA	1.81	0.41
1:B:241:PHE:CZ	1:B:243:ILE:HB	2.56	0.41
1:D:95:GLU:H	1:D:95:GLU:HG3	1.60	0.41
1:B:116:GLU:O	1:B:116:GLU:CG	2.69	0.41
1:B:224:ILE:HB	1:B:227:TYR:HB2	2.02	0.41
1:B:370:ARG:HB3	5:B:653:HOH:O	2.21	0.40
1:C:325:ILE:HD11	1:C:399:ASN:CG	2.47	0.40
1:B:365:PHE:O	1:B:367:ARG:HG3	2.21	0.40
1:D:83:TYR:CE2	1:D:85:PRO:HG3	2.56	0.40
1:A:25:ARG:NH1	1:A:352:GLU:OE1	2.43	0.40
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.85	0.40
1:A:204:ARG:HG2	1:A:204:ARG:HH11	1.86	0.40
1:D:79:LYS:HE3	1:D:79:LYS:HB2	1.51	0.40
1:A:71:VAL:HB	1:A:79:LYS:HB3	2.02	0.40
1:B:60:LEU:HD13	1:B:62:VAL:CB	2.51	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)
5:B:742:HOH:O	5:C:687:HOH:O[15_544]	1.90	0.30
5:C:678:HOH:O	5:D:714:HOH:O[4_555]	1.94	0.26

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	438/448 (98%)	431 (98%)	7 (2%)	0	100	100
1	B	441/448 (98%)	435 (99%)	6 (1%)	0	100	100
1	C	439/448 (98%)	422 (96%)	17 (4%)	0	100	100
1	D	439/448 (98%)	425 (97%)	13 (3%)	1 (0%)	43	56
All	All	1757/1792 (98%)	1713 (98%)	43 (2%)	1 (0%)	48	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	THR

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	378/386 (98%)	369 (98%)	9 (2%)	43	63
1	B	381/386 (99%)	381 (100%)	0	100	100
1	C	379/386 (98%)	373 (98%)	6 (2%)	55	74
1	D	379/386 (98%)	373 (98%)	6 (2%)	55	74
All	All	1517/1544 (98%)	1496 (99%)	21 (1%)	59	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	91	LYS
1	A	92	VAL
1	A	142	SER
1	A	144	MET
1	A	165	LEU
1	A	172	ASN
1	A	282	LEU
1	A	367	ARG
1	C	86	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	134	GLU
1	C	279	GLN
1	C	417	ILE
1	C	418	ARG
1	C	435	ARG
1	D	25	ARG
1	D	31	LEU
1	D	46	MET
1	D	165	LEU
1	D	367	ARG
1	D	381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	221	ASN
1	A	239	HIS
1	B	65	ASN
1	B	172	ASN
1	C	55	GLN
1	C	197	HIS
1	C	376	GLN
1	D	41	GLN
1	D	67	HIS
1	D	111	GLN
1	D	156	HIS
1	D	172	ASN
1	D	197	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	SO4	A	503	-	4,4,4	0.42	0	6,6,6	0.41	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	SO4	1	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	439/448 (97%)	0.52	12 (2%)	56	56	20, 42, 63, 78	1 (0%)
1	B	439/448 (97%)	0.64	22 (5%)	34	34	20, 44, 66, 79	4 (0%)
1	C	439/448 (97%)	0.97	47 (10%)	11	10	22, 54, 77, 97	2 (0%)
1	D	439/448 (97%)	0.71	18 (4%)	41	41	21, 46, 70, 93	2 (0%)
All	All	1756/1792 (97%)	0.71	99 (5%)	30	29	20, 46, 70, 97	9 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90[A]	HIS	4.7
1	D	89	TRP	4.2
1	C	121	TYR	4.2
1	C	439	LEU	4.0
1	D	45	TRP	4.0
1	B	92	VAL	4.0
1	C	343[A]	HIS	3.9
1	B	440	ASP	3.9
1	C	402	PHE	3.9
1	D	439	LEU	3.8
1	B	229[A]	HIS	3.7
1	D	365	PHE	3.7
1	D	236	HIS	3.7
1	B	348	PHE	3.6
1	C	315	LEU	3.5
1	C	313	VAL	3.3
1	C	286	LEU	3.3
1	C	312	ILE	3.3
1	A	111	GLN	3.2
1	C	45	TRP	3.2
1	C	367	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	365	PHE	3.1
1	C	188	ASN	3.1
1	C	440	ASP	3.1
1	D	438	HIS	3.1
1	B	121	TYR	3.1
1	D	86	VAL	3.0
1	C	89	TRP	3.0
1	C	438	HIS	2.9
1	C	398	ASP	2.9
1	D	237	THR	2.9
1	B	118	LEU	2.9
1	A	350	ALA	2.8
1	A	343[A]	HIS	2.8
1	C	229	HIS	2.8
1	C	437	LEU	2.8
1	B	117	LYS	2.7
1	A	89	TRP	2.7
1	D	92	VAL	2.7
1	B	439	LEU	2.7
1	C	92	VAL	2.6
1	D	348	PHE	2.6
1	A	348	PHE	2.6
1	C	403	ILE	2.6
1	C	305	GLN	2.6
1	A	125	ASN	2.6
1	D	93	PRO	2.6
1	C	366	LEU	2.5
1	B	86	VAL	2.5
1	C	91	LYS	2.5
1	D	440	ASP	2.5
1	C	311	ASN	2.5
1	C	362	GLY	2.5
1	C	386	PHE	2.4
1	A	45	TRP	2.4
1	A	438	HIS	2.4
1	C	359	PRO	2.4
1	D	20	ARG	2.4
1	B	116	GLU	2.4
1	D	121	TYR	2.3
1	C	329	PHE	2.3
1	C	28	LEU	2.3
1	A	440	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	45	TRP	2.3
1	C	115	VAL	2.3
1	C	225	LEU	2.2
1	C	384	LEU	2.2
1	C	310	PHE	2.2
1	A	74	GLY	2.2
1	C	264	LYS	2.2
1	B	126	TYR	2.2
1	D	88	PHE	2.2
1	C	317	ALA	2.2
1	B	423	ILE	2.2
1	C	394	LEU	2.2
1	B	228	THR	2.2
1	C	75	ALA	2.2
1	B	188	ASN	2.1
1	C	116	GLU	2.1
1	C	319	ASP	2.1
1	D	114	GLN	2.1
1	C	226	GLY	2.1
1	D	118	LEU	2.1
1	B	343[A]	HIS	2.1
1	C	29	GLU	2.1
1	C	340	LEU	2.1
1	B	93	PRO	2.1
1	A	326	THR	2.0
1	C	277	GLU	2.0
1	B	396	GLN	2.0
1	B	438	HIS	2.0
1	C	236	HIS	2.0
1	C	64	ASP	2.0
1	C	291	LEU	2.0
1	D	417	ILE	2.0
1	B	89	TRP	2.0
1	A	229	HIS	2.0
1	B	367	ARG	2.0
1	C	423	ILE	2.0

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

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	SO4	A	503	5/5	0.82	0.37	30,30,30,30	0
4	NA	A	504	1/1	0.83	0.17	30,30,30,30	0
2	MN	D	501	1/1	0.94	0.10	44,44,44,44	0
2	MN	C	501	1/1	0.95	0.05	52,52,52,52	0
2	MN	A	501	1/1	0.95	0.06	46,46,46,46	0
2	MN	B	501	1/1	0.96	0.05	50,50,50,50	0
2	MN	A	502	1/1	0.96	0.04	50,50,50,50	0
2	MN	C	502	1/1	0.96	0.05	53,53,53,53	0
2	MN	D	502	1/1	0.97	0.09	50,50,50,50	0
2	MN	B	502	1/1	0.98	0.06	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.