



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:46 PM UTC

PDB ID : 7UI1 / pdb_00007ui1
Title : Pfs230 D1D2 domain in complex with 230AL-37
Authors : Tang, W.K.; Tolia, N.H.
Deposited on : 2022-03-28
Resolution : 3.30 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

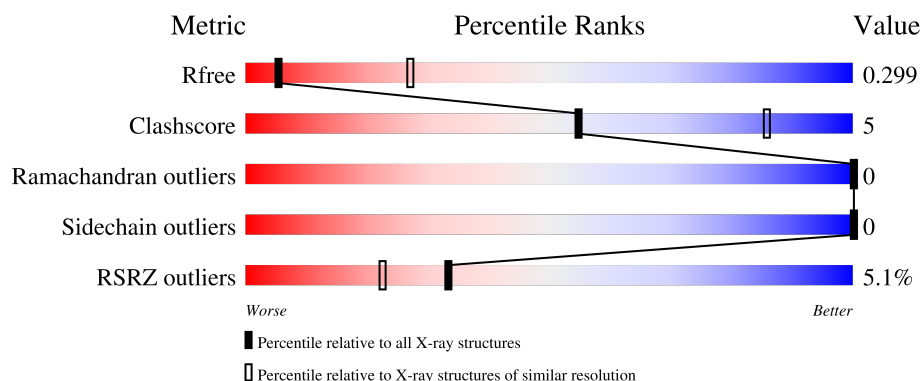
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	355	7% 76% 11% 13%
1	B	355	6% 77% 10% 13%
1	C	355	11% 76% 11% 13%
1	D	355	4% 79% 8% 13%
2	H	257	79% 9% 12%

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Mol	Chain	Length	Quality of chain
2	I	257	77% 12% 12%
2	J	257	2% 75% 14% 12%
2	K	257	77% 11% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34018 atoms, of which 16933 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 Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	0	0
			4984	1604	2495	389	484	12			
1	B	308	Total	C	H	N	O	S	0	0	0
			4982	1604	2493	389	484	12			
1	C	308	Total	C	H	N	O	S	0	0	0
			4983	1604	2494	389	484	12			
1	D	308	Total	C	H	N	O	S	0	0	0
			4983	1604	2494	389	484	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	THR	-	expression tag	UNP P68874
A	541	GLY	-	expression tag	UNP P68874
A	887	GLY	-	expression tag	UNP P68874
A	888	THR	-	expression tag	UNP P68874
A	889	HIS	-	expression tag	UNP P68874
A	890	HIS	-	expression tag	UNP P68874
A	891	HIS	-	expression tag	UNP P68874
A	892	HIS	-	expression tag	UNP P68874
A	893	HIS	-	expression tag	UNP P68874
A	894	HIS	-	expression tag	UNP P68874
B	540	THR	-	expression tag	UNP P68874
B	541	GLY	-	expression tag	UNP P68874
B	887	GLY	-	expression tag	UNP P68874
B	888	THR	-	expression tag	UNP P68874
B	889	HIS	-	expression tag	UNP P68874
B	890	HIS	-	expression tag	UNP P68874
B	891	HIS	-	expression tag	UNP P68874
B	892	HIS	-	expression tag	UNP P68874
B	893	HIS	-	expression tag	UNP P68874
B	894	HIS	-	expression tag	UNP P68874
C	540	THR	-	expression tag	UNP P68874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	541	GLY	-	expression tag	UNP P68874
C	887	GLY	-	expression tag	UNP P68874
C	888	THR	-	expression tag	UNP P68874
C	889	HIS	-	expression tag	UNP P68874
C	890	HIS	-	expression tag	UNP P68874
C	891	HIS	-	expression tag	UNP P68874
C	892	HIS	-	expression tag	UNP P68874
C	893	HIS	-	expression tag	UNP P68874
C	894	HIS	-	expression tag	UNP P68874
D	540	THR	-	expression tag	UNP P68874
D	541	GLY	-	expression tag	UNP P68874
D	887	GLY	-	expression tag	UNP P68874
D	888	THR	-	expression tag	UNP P68874
D	889	HIS	-	expression tag	UNP P68874
D	890	HIS	-	expression tag	UNP P68874
D	891	HIS	-	expression tag	UNP P68874
D	892	HIS	-	expression tag	UNP P68874
D	893	HIS	-	expression tag	UNP P68874
D	894	HIS	-	expression tag	UNP P68874

- Molecule 2 is a protein called 230AL-37.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	227	Total	C	H	N	O	S	0	0	0
			3515	1128	1739	310	333	5			
2	I	227	Total	C	H	N	O	S	0	0	0
			3514	1128	1738	310	333	5			
2	J	227	Total	C	H	N	O	S	0	0	0
			3516	1128	1740	310	333	5			
2	K	227	Total	C	H	N	O	S	0	0	0
			3516	1128	1740	310	333	5			

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

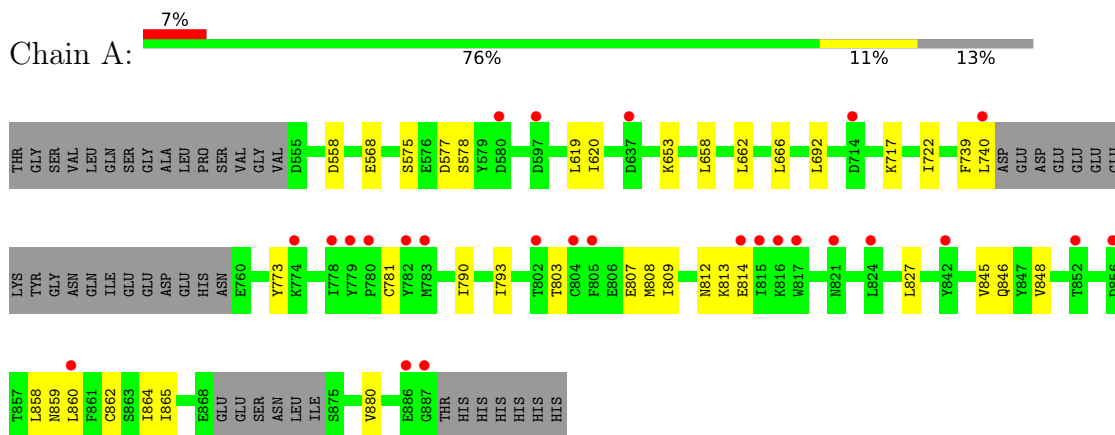


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

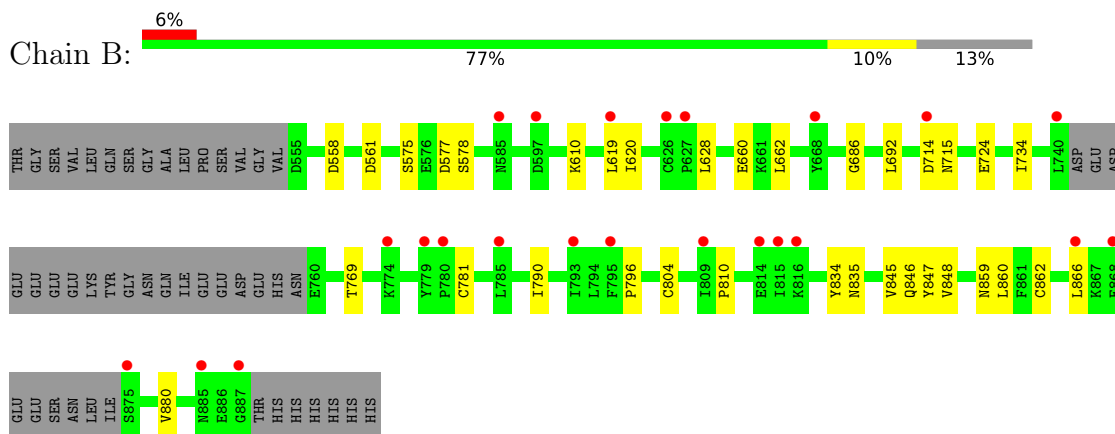
3 Residue-property plots [i](#)

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.

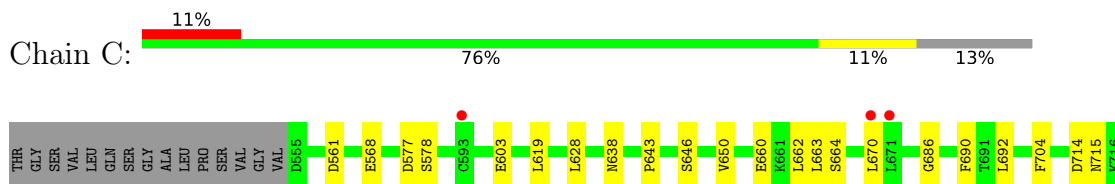
• Molecule 1: Gametocyte surface protein P230

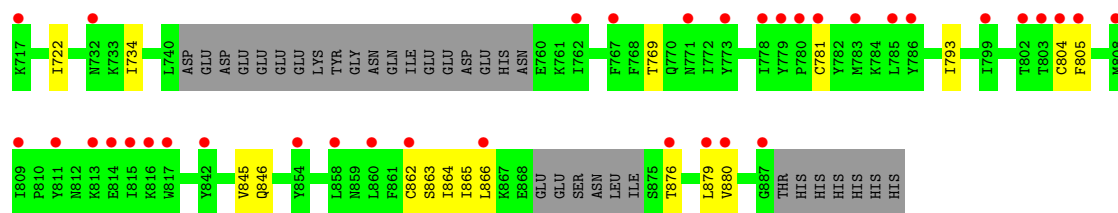


• Molecule 1: Gametocyte surface protein P230

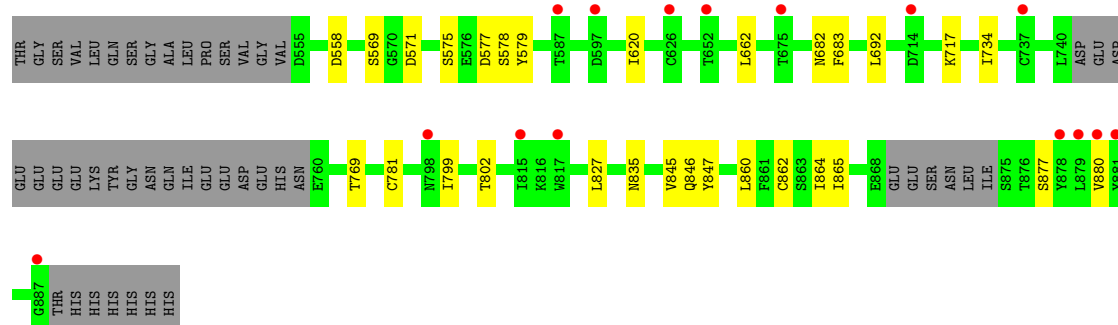
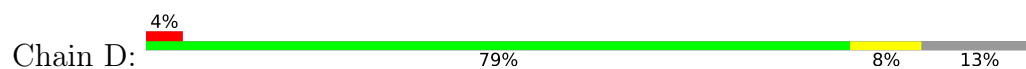


• Molecule 1: Gametocyte surface protein P230

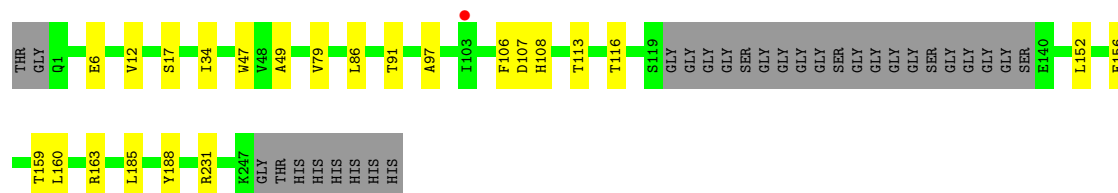
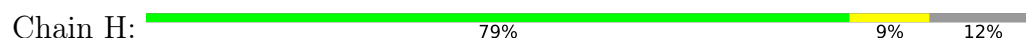




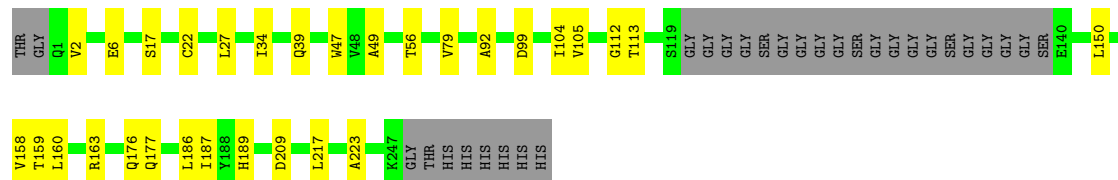
● Molecule 1: Gametocyte surface protein P230



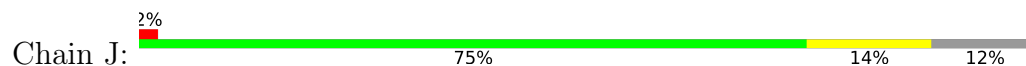
● Molecule 2: 230AL-37



● Molecule 2: 230AL-37



● Molecule 2: 230AL-37



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	49.58Å 155.14Å 375.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 3.30 19.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	77.2 (19.89-3.30) 76.7 (19.89-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.264 , 0.299 0.265 , 0.299	Depositor DCC
R_{free} test set	1717 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	34018	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% 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

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	0.13	0/2538	0.30	0/3425
1	B	0.12	0/2538	0.30	0/3425
1	C	0.13	0/2538	0.31	0/3425
1	D	0.14	0/2538	0.32	0/3425
2	H	0.17	0/1818	0.31	0/2466
2	I	0.19	0/1818	0.33	0/2466
2	J	0.18	0/1818	0.34	0/2466
2	K	0.18	0/1818	0.33	0/2466
All	All	0.15	0/17424	0.32	0/23564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2489	2495	2499	24	0
1	B	2489	2493	2499	22	0
1	C	2489	2494	2499	26	0
1	D	2489	2494	2499	19	0
2	H	1776	1739	1742	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1776	1738	1742	21	1
2	J	1776	1740	1742	28	2
2	K	1776	1740	1742	18	2
3	A	5	0	0	0	0
3	H	10	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
All	All	17085	16933	16964	164	3

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 5.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:12:VAL:HG21	2:J:86:LEU:HD13	1.58	0.84
2:J:101:GLY:O	2:J:102:SER:OG	2.02	0.78
2:I:34:ILE:HG21	2:I:79:VAL:HG11	1.69	0.74
2:K:34:ILE:HG21	2:K:79:VAL:HG11	1.70	0.74
1:A:814:GLU:HG2	1:A:858:LEU:HD12	1.73	0.70
2:J:152:LEU:HD22	2:J:156:GLU:OE1	1.93	0.69
1:D:577:ASP:OD1	1:D:578:SER:N	2.28	0.67
1:B:796:PRO:HG2	1:B:866:LEU:HD21	1.77	0.66
2:H:152:LEU:HD22	2:H:156:GLU:OE1	1.95	0.65
2:J:34:ILE:HG21	2:J:79:VAL:HG11	1.80	0.64
1:C:781:CYS:SG	1:C:880:VAL:HG13	2.38	0.63
1:B:558:ASP:HB2	1:B:662:LEU:HD21	1.80	0.62
1:D:682:ASN:OD1	1:D:683:PHE:N	2.33	0.61
1:C:714:ASP:OD2	2:J:52:ARG:NE	2.34	0.61
1:A:577:ASP:OD1	1:A:578:SER:N	2.35	0.60
1:B:610:LYS:NZ	1:B:724:GLU:OE1	2.24	0.60
1:A:781:CYS:HB3	1:A:880:VAL:HG22	1.84	0.59
1:A:808:MET:HB2	1:A:827:LEU:HD11	1.83	0.59
1:C:603:GLU:OE2	1:C:715:ASN:ND2	2.36	0.58
1:B:577:ASP:OD1	1:B:578:SER:N	2.36	0.58
1:C:577:ASP:OD1	1:C:578:SER:N	2.37	0.58
2:K:141:ILE:O	2:K:237:THR:HG21	2.02	0.58
2:H:34:ILE:HG21	2:H:79:VAL:HG11	1.87	0.57
2:J:12:VAL:HG21	2:J:86:LEU:CD1	2.33	0.57
1:C:561:ASP:N	1:C:660:GLU:OE1	2.35	0.57
1:A:662:LEU:O	1:A:666:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:ASN:O	1:B:860:LEU:HD23	2.05	0.56
1:D:717:LYS:HZ1	2:K:231:ARG:HA	1.69	0.56
2:K:140:GLU:OE1	2:K:232:ASN:ND2	2.38	0.56
1:C:650:VAL:HG12	1:C:704:PHE:CZ	2.42	0.55
2:J:99:ASP:OD1	2:J:100:ARG:N	2.40	0.55
1:A:781:CYS:SG	1:A:880:VAL:HG13	2.48	0.53
1:A:740:LEU:HD12	1:A:773:TYR:CE1	2.44	0.53
1:B:734:ILE:O	1:B:769:THR:HG23	2.09	0.53
1:B:620:ILE:HB	1:B:692:LEU:HD12	1.92	0.52
2:I:56:THR:HB	2:J:56:THR:HB	1.92	0.52
1:A:558:ASP:HB2	1:A:662:LEU:HD21	1.90	0.52
2:K:2:VAL:HG13	2:K:27:LEU:HD23	1.91	0.52
1:C:662:LEU:HD22	1:C:664:SER:OG	2.10	0.52
1:D:558:ASP:HB2	1:D:662:LEU:HD21	1.92	0.51
1:C:804:CYS:HA	1:C:862:CYS:HB2	1.92	0.51
2:H:185:LEU:HD21	2:H:188:TYR:HB3	1.92	0.50
1:C:793:ILE:HD12	1:C:805:PHE:CZ	2.46	0.50
1:A:575:SER:OG	1:A:577:ASP:OD1	2.26	0.50
1:A:808:MET:HE1	1:A:862:CYS:SG	2.51	0.50
2:H:91:THR:HG23	2:H:116:THR:HA	1.93	0.50
1:C:793:ILE:HD12	1:C:805:PHE:HZ	1.76	0.49
1:A:620:ILE:HB	1:A:692:LEU:HD12	1.95	0.49
1:C:862:CYS:SG	1:C:880:VAL:HB	2.52	0.49
1:C:638:ASN:OD1	2:J:102:SER:OG	2.28	0.48
1:D:799:ILE:HD11	1:D:802:THR:HB	1.95	0.48
1:C:781:CYS:HB3	1:C:880:VAL:HG22	1.94	0.48
1:C:734:ILE:O	1:C:769:THR:HG23	2.12	0.48
1:D:620:ILE:HB	1:D:692:LEU:HD12	1.95	0.48
1:B:835:ASN:ND2	1:B:845:VAL:O	2.42	0.48
2:I:6:GLU:N	2:I:6:GLU:OE2	2.47	0.48
1:B:810:PRO:HB3	1:B:860:LEU:HD22	1.95	0.47
1:B:619:LEU:HD13	1:B:834:TYR:CE2	2.50	0.47
2:I:39:GLN:C	2:I:92:ALA:HB1	2.39	0.47
1:B:575:SER:OG	1:B:577:ASP:OD1	2.31	0.47
1:D:575:SER:OG	1:D:577:ASP:OD1	2.31	0.47
2:J:159:THR:C	2:J:160:LEU:HD12	2.40	0.47
2:K:39:GLN:OE1	2:K:177:GLN:NE2	2.42	0.47
2:K:113:THR:HG23	2:K:113:THR:O	2.13	0.47
2:J:200:ARG:HD2	2:J:216:SER:O	2.15	0.47
1:D:835:ASN:ND2	1:D:845:VAL:O	2.42	0.47
2:K:159:THR:C	2:K:160:LEU:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ILE:HG23	1:A:848:VAL:O	2.15	0.46
2:I:187:ILE:HG22	2:I:189:HIS:O	2.15	0.46
2:K:12:VAL:HG21	2:K:86:LEU:HD13	1.98	0.46
1:A:717:LYS:HE2	2:H:231:ARG:HA	1.97	0.46
2:J:163:ARG:HB3	2:J:163:ARG:NH2	2.30	0.46
1:D:864:ILE:HG22	1:D:865:ILE:N	2.31	0.46
1:C:863:SER:HA	1:C:879:LEU:HD23	1.97	0.46
2:H:152:LEU:HD11	2:I:163:ARG:CZ	2.45	0.46
1:C:866:LEU:HD12	1:C:876:THR:O	2.16	0.46
1:C:568:GLU:O	1:C:722:ILE:HD11	2.16	0.46
1:A:808:MET:O	1:A:809:ILE:HD13	2.15	0.46
1:C:670:LEU:HD21	1:C:690:PHE:HD2	1.81	0.45
1:D:862:CYS:SG	1:D:880:VAL:HB	2.56	0.45
2:K:35:TYR:HE1	2:K:99:ASP:HB3	1.81	0.45
2:J:6:GLU:OE1	2:J:112:GLY:N	2.48	0.45
2:H:6:GLU:N	2:H:6:GLU:OE1	2.49	0.45
2:J:35:TYR:OH	2:J:104:ILE:HD12	2.16	0.45
1:B:790:ILE:HG23	1:B:848:VAL:O	2.17	0.45
1:C:643:PRO:O	1:C:646:SER:OG	2.29	0.45
1:C:662:LEU:HD23	1:C:663:LEU:N	2.31	0.45
2:H:159:THR:N	2:I:209:ASP:OD2	2.49	0.45
2:I:22:CYS:HB3	2:I:79:VAL:HG13	1.98	0.45
2:J:228:GLN:HG2	2:J:229:GLN:N	2.30	0.45
2:I:99:ASP:HA	2:I:105:VAL:O	2.16	0.44
2:I:47:TRP:NE1	2:I:49:ALA:O	2.50	0.44
2:J:170:ILE:HA	2:J:190:VAL:HG23	1.99	0.44
2:J:101:GLY:O	2:J:102:SER:CB	2.65	0.44
2:H:159:THR:C	2:H:160:LEU:HD12	2.43	0.44
2:I:2:VAL:HG13	2:I:27:LEU:HD23	1.98	0.44
2:K:39:GLN:C	2:K:92:ALA:HB1	2.43	0.44
2:H:152:LEU:HD11	2:I:163:ARG:NH1	2.33	0.44
1:B:781:CYS:HB3	1:B:880:VAL:HG22	1.99	0.44
1:D:569:SER:OG	1:D:579:TYR:OH	2.22	0.43
2:J:2:VAL:HG13	2:J:27:LEU:HD23	2.00	0.43
2:I:104:ILE:O	2:I:104:ILE:HG22	2.17	0.43
2:I:158:VAL:HG21	2:I:217:LEU:HD11	2.00	0.43
1:B:628:LEU:HD21	1:B:686:GLY:CA	2.48	0.43
2:K:187:ILE:HG22	2:K:189:HIS:O	2.17	0.43
2:J:187:ILE:HG22	2:J:189:HIS:O	2.19	0.43
2:K:35:TYR:CE1	2:K:99:ASP:HB3	2.54	0.43
1:D:845:VAL:HG11	1:D:847:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:159:THR:C	2:I:160:LEU:HD12	2.44	0.43
2:K:160:LEU:HD12	2:K:160:LEU:N	2.33	0.43
1:B:561:ASP:N	1:B:660:GLU:OE1	2.48	0.43
2:I:6:GLU:OE1	2:I:112:GLY:N	2.49	0.43
2:I:177:GLN:O	2:I:223:ALA:HB1	2.19	0.43
2:J:160:LEU:HD12	2:J:160:LEU:N	2.34	0.43
2:H:163:ARG:HD2	2:I:150:LEU:HD21	2.01	0.42
1:B:714:ASP:O	2:I:104:ILE:HD11	2.18	0.42
1:B:845:VAL:HG12	1:B:846:GLN:N	2.35	0.42
2:J:152:LEU:HD13	2:J:156:GLU:HB2	2.00	0.42
2:J:168:VAL:HG21	2:J:172:LEU:HD12	2.00	0.42
2:H:47:TRP:NE1	2:H:49:ALA:O	2.51	0.42
1:D:845:VAL:HG12	1:D:846:GLN:N	2.34	0.42
1:A:812:ASN:O	1:A:813:LYS:HG3	2.18	0.42
2:J:35:TYR:HE1	2:J:99:ASP:HB2	1.84	0.42
2:J:141:ILE:HD11	2:J:232:ASN:HB3	2.01	0.42
2:J:170:ILE:HA	2:J:190:VAL:CG2	2.49	0.42
2:K:151:SER:O	2:K:152:LEU:HD23	2.19	0.42
1:A:619:LEU:HD12	1:A:790:ILE:HD13	2.00	0.42
1:D:827:LEU:HD13	1:D:860:LEU:HD13	2.01	0.42
2:J:172:LEU:HD23	2:J:173:ALA:N	2.35	0.42
1:A:739:PHE:HE1	1:A:793:ILE:HG23	1.83	0.42
2:H:160:LEU:HD12	2:H:160:LEU:N	2.35	0.42
2:I:176:GLN:HB2	2:I:186:LEU:HD11	2.00	0.42
2:J:27:LEU:C	2:J:27:LEU:HD12	2.45	0.42
1:D:734:ILE:O	1:D:769:THR:HG23	2.19	0.42
1:A:803:THR:HB	1:A:807:GLU:HB2	2.01	0.42
1:A:859:ASN:O	1:A:860:LEU:HD23	2.20	0.42
1:D:781:CYS:HB3	1:D:880:VAL:HA	2.02	0.42
1:D:781:CYS:SG	1:D:880:VAL:HG13	2.60	0.42
1:D:864:ILE:O	1:D:877:SER:CB	2.68	0.42
1:A:568:GLU:O	1:A:722:ILE:HD11	2.20	0.41
2:H:107:ASP:OD1	2:H:108:HIS:N	2.50	0.41
1:B:845:VAL:HG11	1:B:847:TYR:CZ	2.55	0.41
1:B:804:CYS:HA	1:B:862:CYS:HB2	2.02	0.41
1:C:619:LEU:HD23	1:C:692:LEU:O	2.20	0.41
1:C:670:LEU:CD1	1:C:692:LEU:HD23	2.50	0.41
1:A:864:ILE:HG22	1:A:865:ILE:N	2.36	0.41
1:B:862:CYS:SG	1:B:880:VAL:HB	2.61	0.41
2:I:113:THR:O	2:I:113:THR:HG23	2.21	0.41
1:C:628:LEU:HD21	1:C:686:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:VAL:HG12	1:A:846:GLN:N	2.35	0.41
1:B:715:ASN:OD1	1:B:715:ASN:N	2.47	0.41
2:H:12:VAL:HG21	2:H:86:LEU:HD13	2.03	0.41
1:C:864:ILE:HG22	1:C:865:ILE:N	2.36	0.41
1:D:571:ASP:HB3	2:K:170:ILE:HG21	2.03	0.41
1:C:845:VAL:HG12	1:C:846:GLN:N	2.36	0.41
2:H:97:ALA:HB1	2:H:106:PHE:HB3	2.03	0.40
2:J:189:HIS:O	2:J:190:VAL:C	2.65	0.40
1:A:619:LEU:HD23	1:A:692:LEU:O	2.21	0.40
1:B:628:LEU:HD21	1:B:686:GLY:N	2.37	0.40
1:C:670:LEU:HD21	1:C:690:PHE:CD2	2.56	0.40
1:A:653:LYS:HA	1:A:658:LEU:HD23	2.03	0.40
2:H:113:THR:O	2:H:113:THR:HG23	2.20	0.40
2:K:63:SER:O	2:K:67:ARG:NH2	2.54	0.40
2:K:163:ARG:CZ	2:K:163:ARG:HB3	2.52	0.40

All (3) 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)
2:J:17:SER:H	2:K:17:SER:OG[3_555]	1.47	0.13
2:J:159:THR:N	2:K:209:ASP:OD2[1_655]	2.17	0.03
2:H:17:SER:OG	2:I:17:SER:O[3_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/355 (85%)	283 (94%)	19 (6%)	0	100	100
1	B	302/355 (85%)	289 (96%)	13 (4%)	0	100	100
1	C	302/355 (85%)	285 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	302/355 (85%)	285 (94%)	17 (6%)	0	100	100
2	H	223/257 (87%)	216 (97%)	7 (3%)	0	100	100
2	I	223/257 (87%)	216 (97%)	7 (3%)	0	100	100
2	J	223/257 (87%)	213 (96%)	10 (4%)	0	100	100
2	K	223/257 (87%)	215 (96%)	8 (4%)	0	100	100
All	All	2100/2448 (86%)	2002 (95%)	98 (5%)	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	289/331 (87%)	289 (100%)	0	100	100
1	B	289/331 (87%)	289 (100%)	0	100	100
1	C	289/331 (87%)	289 (100%)	0	100	100
1	D	289/331 (87%)	289 (100%)	0	100	100
2	H	191/203 (94%)	191 (100%)	0	100	100
2	I	191/203 (94%)	191 (100%)	0	100	100
2	J	191/203 (94%)	191 (100%)	0	100	100
2	K	191/203 (94%)	191 (100%)	0	100	100
All	All	1920/2136 (90%)	1920 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	798	ASN
2	H	74	ASN
2	H	108	HIS

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Mol	Chain	Res	Type
1	B	598	GLN
1	B	697	HIS
2	I	1	GLN
1	C	588	ASN
2	J	84	ASN
2	J	166	GLN
1	D	638	ASN
1	D	859	ASN
2	K	39	GLN
2	K	74	ASN
2	K	177	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	K	301	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	H	302	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	J	301	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	H	301	-	4,4,4	0.22	0	6,6,6	0.19	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	308/355 (86%)	0.76	26 (8%) 17 13	48, 138, 229, 265	0
1	B	308/355 (86%)	0.69	23 (7%) 20 15	51, 136, 225, 281	0
1	C	308/355 (86%)	0.92	39 (12%) 8 6	58, 137, 253, 312	0
1	D	308/355 (86%)	0.55	15 (4%) 35 23	49, 110, 195, 280	0
2	H	227/257 (88%)	0.24	1 (0%) 88 79	34, 56, 88, 124	0
2	I	227/257 (88%)	0.17	0 100 100	29, 48, 73, 96	0
2	J	227/257 (88%)	0.21	4 (1%) 67 49	33, 50, 69, 93	0
2	K	227/257 (88%)	0.26	1 (0%) 88 79	32, 54, 78, 142	0
All	All	2140/2448 (87%)	0.51	109 (5%) 33 22	29, 81, 220, 312	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	779	TYR	5.3
1	A	804	CYS	4.9
1	A	815	ILE	4.6
1	C	887	GLY	4.3
1	C	780	PRO	4.0
1	A	580	ASP	3.8
1	C	815	ILE	3.8
1	A	805	PHE	3.6
1	C	811	TYR	3.5
1	A	814	GLU	3.5
1	B	795	PHE	3.4
1	C	767	PHE	3.4
1	C	804	CYS	3.4
1	C	880	VAL	3.4
1	B	887	GLY	3.4
1	C	799	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	714	ASP	3.2
1	B	793	ILE	3.2
1	C	813	LYS	3.1
1	A	852	THR	3.0
1	A	816	LYS	3.0
1	D	714	ASP	3.0
1	C	771	ASN	3.0
1	D	878	TYR	3.0
2	J	99	ASP	3.0
1	C	805	PHE	2.9
1	A	824	LEU	2.9
1	D	815	ILE	2.9
1	C	876	THR	2.9
1	A	780	PRO	2.9
1	B	814	GLU	2.9
1	B	816	LYS	2.9
1	A	783	MET	2.8
1	C	862	CYS	2.8
1	A	802	THR	2.8
1	C	809	ILE	2.8
1	D	587	THR	2.8
1	D	887	GLY	2.7
1	C	670	LEU	2.7
1	A	887	GLY	2.7
1	B	868	GLU	2.7
1	B	585	ASN	2.7
1	D	881	TYR	2.6
1	C	671	LEU	2.6
1	D	817	TRP	2.6
1	C	814	GLU	2.6
1	A	637	ASP	2.6
1	A	856	ASP	2.6
1	C	762	ILE	2.5
1	B	619	LEU	2.5
1	D	675	THR	2.5
2	J	222	PHE	2.5
1	A	842	TYR	2.5
1	B	740	LEU	2.5
1	D	798	ASN	2.5
1	C	817	TRP	2.5
1	A	782	TYR	2.5
1	C	781	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	593	CYS	2.4
1	C	858	LEU	2.4
1	A	821	ASN	2.4
2	H	103	ILE	2.4
1	C	717	LYS	2.4
1	B	885	ASN	2.3
1	B	774	LYS	2.3
1	B	626	CYS	2.3
1	C	783	MET	2.3
1	D	880	VAL	2.3
1	C	816	LYS	2.3
1	C	778	ILE	2.3
2	K	188	TYR	2.3
1	B	866	LEU	2.3
1	C	860	LEU	2.3
1	B	668	TYR	2.2
1	C	842	TYR	2.2
1	D	597	ASP	2.2
1	C	802	THR	2.2
1	C	803	THR	2.2
1	D	626	CYS	2.2
1	B	627	PRO	2.2
1	C	866	LEU	2.2
1	A	817	TRP	2.2
1	B	815	ILE	2.2
1	C	773	TYR	2.2
1	B	809	ILE	2.2
2	J	202	SER	2.2
1	B	714	ASP	2.2
1	C	785	LEU	2.1
1	B	780	PRO	2.1
1	C	854	TYR	2.1
1	B	875	SER	2.1
1	A	774	LYS	2.1
1	A	779	TYR	2.1
1	C	879	LEU	2.1
1	C	732	ASN	2.1
1	B	597	ASP	2.1
1	B	779	TYR	2.1
1	C	808	MET	2.1
2	J	101	GLY	2.1
1	A	886	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	597	ASP	2.0
1	C	786	TYR	2.0
1	A	860	LEU	2.0
1	D	652	THR	2.0
1	D	737	CYS	2.0
1	A	740	LEU	2.0
1	B	785	LEU	2.0
1	D	879	LEU	2.0
1	A	778	ILE	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	SO4	K	301	5/5	0.79	0.14	61,66,68,73	0
3	SO4	H	302	5/5	0.81	0.09	68,68,74,74	0
3	SO4	H	301	5/5	0.89	0.11	54,56,59,61	0
3	SO4	J	301	5/5	0.93	0.06	57,58,59,61	0
3	SO4	A	901	5/5	0.95	0.08	56,56,59,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.