



# Full wwPDB X-ray Structure Validation Report i

Oct 15, 2023 – 05:57 AM EDT

PDB ID : 7UI1  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

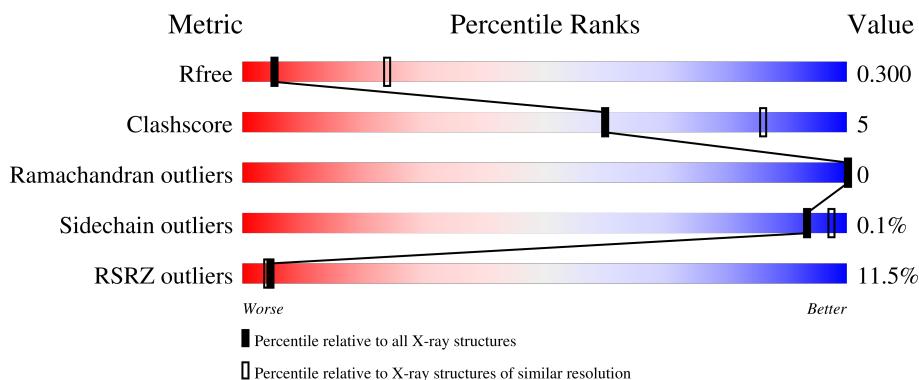
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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.



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

## 2 Entry composition i

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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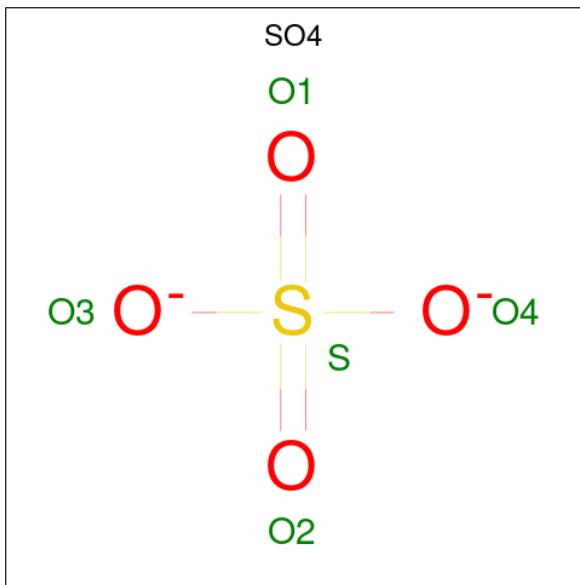
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Chain	Residue	Modelled	Actual	Comment	Reference
C	541	GLY	-	expression tag	UNP P68874
C	887	GLY	-	expression tag	UNP P68874
C	888	THR	-	expression tag	UNP P68874
C	889	HIS	-	expression tag	UNP P68874
C	890	HIS	-	expression tag	UNP P68874
C	891	HIS	-	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 (three-letter code: SO4) (formula: O<sub>4</sub>S).

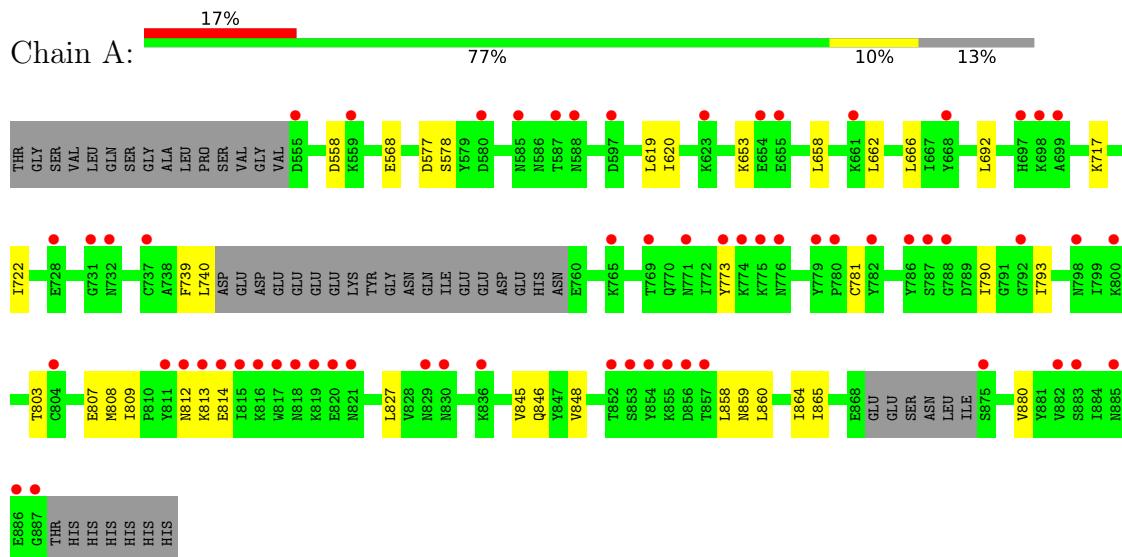


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

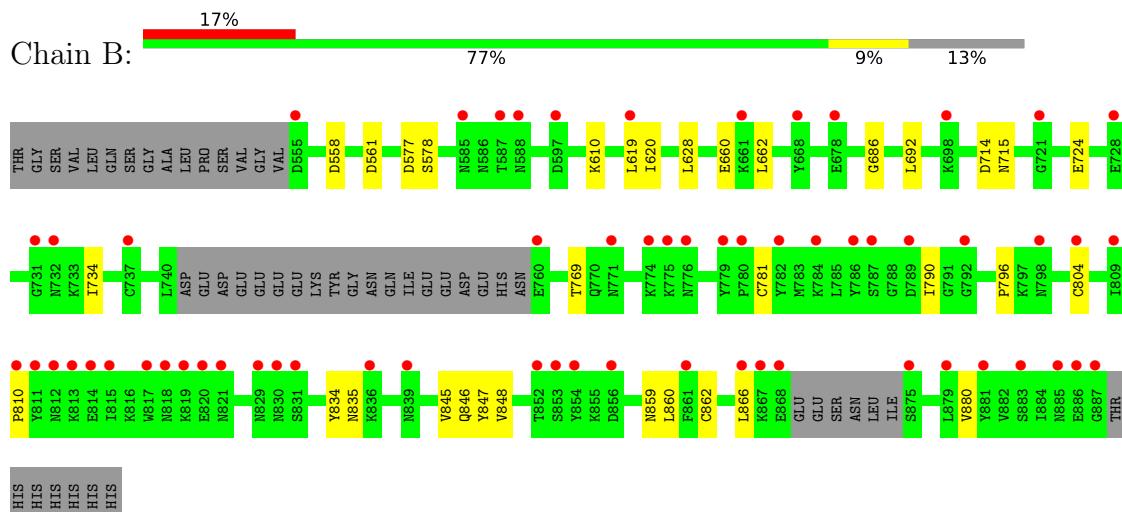
### 3 Residue-property plots

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.

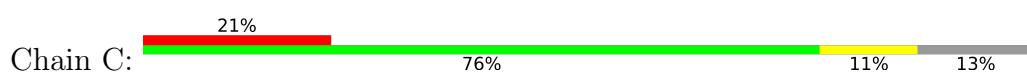
- Molecule 1: Gametocyte surface protein P230



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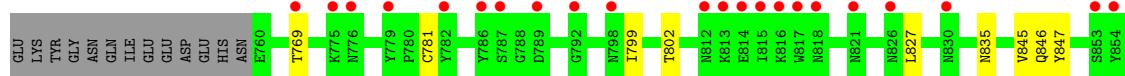
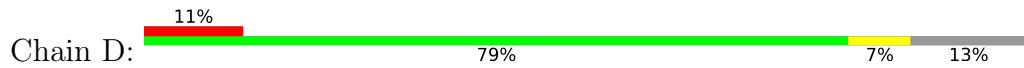


- Molecule 1: Gametocyte surface protein P230

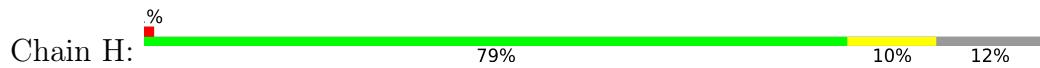




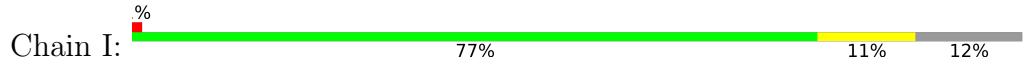
- Molecule 1: Gametocyte surface protein P230



- Molecule 2: 230AL-37



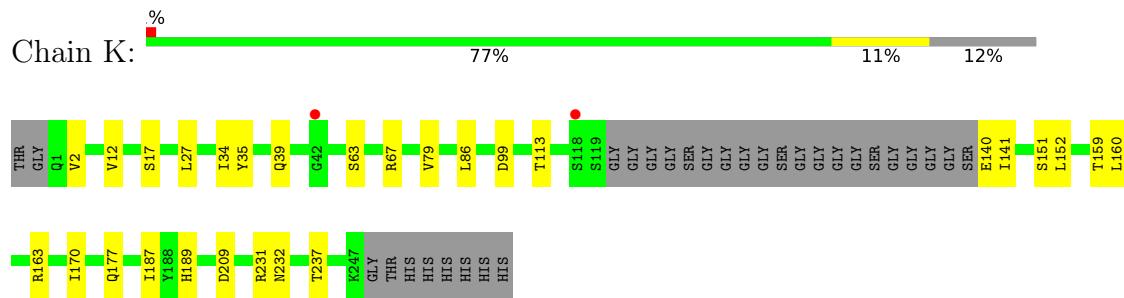
- Molecule 2: 230AL-37



- Molecule 2: 230AL-37



- Molecule 2: 230AL-37



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 1 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.58 Å   155.14 Å   375.22 Å 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) 77.3 (19.89-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.54 (at 3.29 Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
$R$ , $R_{free}$	0.264 , 0.299 0.264 , 0.300	Depositor DCC
$R_{free}$ test set	1717 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.47$ , $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	34018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  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	0.26	0/2538	0.46	0/3425
1	B	0.26	0/2538	0.46	0/3425
1	C	0.26	0/2538	0.47	0/3425
1	D	0.27	0/2538	0.47	0/3425
2	H	0.30	0/1818	0.52	0/2466
2	I	0.31	0/1818	0.53	0/2466
2	J	0.31	0/1818	0.54	0/2466
2	K	0.31	0/1818	0.53	0/2466
All	All	0.28	0/17424	0.49	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	22	0
1	B	2489	2493	2499	21	0
1	C	2489	2494	2499	25	0
1	D	2489	2494	2499	18	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	20	1
2	J	1776	1740	1742	26	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	155	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 (155) 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
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:D:717:LYS:HZ1	2:K:231:ARG:HA	1.72	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
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:K:113:THR:HG23	2:K:113:THR:O	2.13	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:K:39:GLN:OE1	2:K:177:GLN:NE2	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:2:VAL:HG13	2:I:27:LEU:HD23	1.98	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
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
2:I:39:GLN:C	2:I:92:ALA:HB1	2.39	0.43
1:D:845:VAL:HG11	1:D:847:TYR:CZ	2.54	0.43
2:K:160:LEU:N	2:K:160:LEU:HD12	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
1:D:845:VAL:HG12	1:D:846:GLN:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:812:ASN:O	1:A:813:LYS:HG3	2.18	0.42
2:H:20:LEU:HD11	2:H:83:MET:HE1	2.01	0.42
2:J:159:THR:C	2:J:160:LEU:HD12	2.40	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
2:K:159:THR:C	2:K:160:LEU:HD12	2.40	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
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
1:A:845:VAL:HG12	1:A:846:GLN:N	2.35	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
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:D:717:LYS:NZ	2:K:231:ARG:HA	2.36	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
1:A:619:LEU:HD23	1:A:692:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

### 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	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
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 [\(i\)](#)

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%)	288 (100%)	1 (0%)	92 96
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%)	1919 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	782	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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	H	302	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	K	301	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	J	301	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	H	301	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.11	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	308/355 (86%)	1.27	62 (20%) 1   1	44, 127, 208, 239	0
1	B	308/355 (86%)	1.19	62 (20%) 1   1	47, 125, 204, 260	0
1	C	308/355 (86%)	1.33	75 (24%) 0   0	54, 125, 232, 277	0
1	D	308/355 (86%)	0.80	40 (12%) 3   3	46, 99, 178, 247	0
2	H	227/257 (88%)	0.07	3 (1%) 77   77	30, 51, 78, 109	0
2	I	227/257 (88%)	-0.06	2 (0%) 84   84	27, 43, 65, 87	0
2	J	227/257 (88%)	-0.02	0 100   100	31, 45, 63, 82	0
2	K	227/257 (88%)	0.06	2 (0%) 84   84	29, 50, 70, 122	0
All	All	2140/2448 (87%)	0.67	246 (11%) 4   4	27, 74, 201, 277	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	814	GLU	10.6
1	A	821	ASN	10.6
1	A	855	LYS	10.0
1	D	813	LYS	9.6
1	A	775	LYS	9.3
1	D	817	TRP	9.2
1	C	817	TRP	8.9
1	C	821	ASN	8.6
1	B	787	SER	8.3
1	A	817	TRP	8.0
1	B	853	SER	7.8
1	B	775	LYS	7.7
1	C	776	ASN	7.6
1	C	814	GLU	7.6
1	A	780	PRO	7.6
1	C	853	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	815	ILE	7.1
1	B	817	TRP	7.1
1	C	813	LYS	7.0
1	B	885	ASN	6.9
1	B	731	GLY	6.9
1	A	779	TYR	6.6
1	A	776	ASN	6.4
1	A	887	GLY	6.4
1	A	829	ASN	6.4
1	B	814	GLU	6.3
1	B	830	ASN	6.1
1	C	769	THR	6.0
1	C	732	ASN	6.0
1	B	776	ASN	6.0
1	C	775	LYS	5.9
1	B	820	GLU	5.9
1	C	820	GLU	5.7
1	C	852	THR	5.7
1	C	812	ASN	5.6
1	D	815	ILE	5.6
1	A	774	LYS	5.5
1	A	820	GLU	5.5
1	C	815	ILE	5.4
1	B	821	ASN	5.4
1	A	856	ASP	5.3
1	D	798	ASN	5.2
1	A	782	TYR	5.2
1	A	853	SER	5.1
1	A	798	ASN	5.1
1	C	816	LYS	5.1
1	C	887	GLY	5.1
1	A	811	TYR	5.1
1	D	814	GLU	5.0
1	C	788	GLY	5.0
1	A	588	ASN	5.0
1	C	799	ILE	5.0
1	A	555	ASP	4.9
1	C	786	TYR	4.9
1	C	588	ASN	4.9
1	C	831	SER	4.8
1	D	816	LYS	4.8
1	A	787	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	587	THR	4.8
1	A	732	ASN	4.8
1	A	857	THR	4.8
1	B	779	TYR	4.8
1	B	818	ASN	4.7
1	A	816	LYS	4.7
1	C	830	ASN	4.7
1	D	886	GLU	4.7
1	B	587	THR	4.6
1	A	818	ASN	4.6
1	C	731	GLY	4.6
1	C	773	TYR	4.6
1	C	854	TYR	4.6
1	B	555	ASP	4.6
1	C	822	LYS	4.5
1	B	780	PRO	4.4
1	C	780	PRO	4.4
1	C	826	ASN	4.4
1	C	855	LYS	4.4
1	C	862	CYS	4.4
1	B	810	PRO	4.4
1	A	813	LYS	4.4
1	A	769	THR	4.3
1	B	815	ILE	4.3
1	B	831	SER	4.2
1	C	587	THR	4.1
1	B	852	THR	4.1
1	C	782	TYR	4.0
1	A	792	GLY	4.0
1	A	886	GLU	4.0
1	A	804	CYS	4.0
1	B	829	ASN	4.0
1	A	661	LYS	3.9
1	D	853	SER	3.9
1	A	786	TYR	3.9
1	A	773	TYR	3.9
1	C	729	PRO	3.9
1	D	782	TYR	3.9
1	C	661	LYS	3.8
1	C	656	THR	3.8
1	D	654	GLU	3.7
1	C	818	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	588	ASN	3.7
1	B	887	GLY	3.7
1	A	830	ASN	3.7
1	B	732	ASN	3.7
1	C	881	TYR	3.7
2	I	119	SER	3.6
1	B	861	PHE	3.6
1	D	812	ASN	3.6
1	A	883	SER	3.5
1	C	771	ASN	3.5
1	D	732	ASN	3.5
1	C	868	GLU	3.5
1	B	786	TYR	3.5
1	A	655	GLU	3.4
1	C	779	TYR	3.4
1	B	866	LEU	3.4
2	H	119	SER	3.4
1	C	876	THR	3.4
1	C	555	ASP	3.3
1	B	737	CYS	3.3
1	B	792	GLY	3.3
1	A	852	THR	3.3
1	A	800	LYS	3.2
1	B	881	TYR	3.2
1	C	762	ILE	3.2
1	C	857	THR	3.2
1	A	698	LYS	3.2
1	B	812	ASN	3.2
1	B	811	TYR	3.1
1	D	818	ASN	3.1
1	A	885	ASN	3.1
1	A	771	ASN	3.1
1	C	807	GLU	3.1
1	D	876	THR	3.1
1	B	868	GLU	3.1
1	C	829	ASN	3.1
2	H	1	GLN	3.0
1	C	604	SER	3.0
1	A	587	THR	3.0
1	D	776	ASN	2.9
1	D	677	ASN	2.9
1	D	855	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	830	ASN	2.9
1	B	782	TYR	2.9
1	B	784	LYS	2.9
1	B	804	CYS	2.9
1	A	882	VAL	2.9
1	D	881	TYR	2.9
1	C	819	LYS	2.9
1	C	867	LYS	2.9
1	D	868	GLU	2.9
1	D	821	ASN	2.9
1	B	813	LYS	2.9
1	D	786	TYR	2.8
1	B	809	ILE	2.8
1	B	819	LYS	2.8
1	C	772	ILE	2.8
1	C	781	CYS	2.8
1	A	585	ASN	2.8
1	C	721	GLY	2.8
1	B	668	TYR	2.8
2	K	42	GLY	2.8
1	A	819	LYS	2.8
1	C	668	TYR	2.8
1	B	839	ASN	2.8
1	D	859	ASN	2.8
1	D	775	LYS	2.8
1	A	812	ASN	2.8
1	B	774	LYS	2.7
1	D	779	TYR	2.7
1	C	765	LYS	2.7
1	B	798	ASN	2.7
1	C	778	ILE	2.7
1	D	588	ASN	2.7
1	A	728	GLU	2.7
1	B	760	GLU	2.7
2	H	118	SER	2.6
1	A	737	CYS	2.6
1	A	875	SER	2.6
1	C	787	SER	2.6
1	D	789	ASP	2.6
1	C	603	GLU	2.6
1	A	765	LYS	2.6
1	C	774	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	771	ASN	2.5
1	C	837	GLU	2.5
1	C	789	ASP	2.5
1	D	878	TYR	2.5
1	B	698	LYS	2.5
1	C	800	LYS	2.5
1	D	629	LYS	2.5
1	B	619	LEU	2.5
1	D	737	CYS	2.4
1	A	731	GLY	2.4
1	A	788	GLY	2.4
1	D	877	SER	2.4
1	C	655	GLU	2.4
1	C	777	ASN	2.4
1	B	867	LYS	2.4
1	C	737	CYS	2.4
1	C	697	HIS	2.4
1	C	556	GLU	2.3
1	D	826	ASN	2.3
1	A	597	ASP	2.3
1	B	585	ASN	2.3
1	A	559	LYS	2.3
1	B	678	GLU	2.3
1	D	655	GLU	2.3
1	A	668	TYR	2.3
1	B	854	TYR	2.3
1	B	661	LYS	2.3
1	C	726	TYR	2.3
1	C	792	GLY	2.3
1	C	832	VAL	2.3
1	D	792	GLY	2.2
1	B	883	SER	2.2
1	C	863	SER	2.2
1	D	555	ASP	2.2
1	C	841	LYS	2.2
1	C	886	GLU	2.2
1	B	721	GLY	2.2
1	A	854	TYR	2.2
1	B	875	SER	2.2
1	C	866	LEU	2.2
1	A	580	ASP	2.1
1	B	597	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	811	TYR	2.1
1	A	697	HIS	2.1
1	B	728	GLU	2.1
1	D	726	TYR	2.1
1	B	856	ASP	2.1
2	I	240	GLN	2.1
1	D	769	THR	2.1
1	B	836	LYS	2.1
1	A	699	ALA	2.1
1	B	789	ASP	2.1
1	C	698	LYS	2.1
1	D	854	TYR	2.0
1	C	810	PRO	2.0
1	A	623	LYS	2.0
1	A	836	LYS	2.0
1	D	787	SER	2.0
2	K	118	SER	2.0
1	B	886	GLU	2.0
1	A	654	GLU	2.0
1	B	879	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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	H	302	5/5	0.91	0.18	68,68,74,74	0
3	SO4	K	301	5/5	0.93	0.24	61,66,68,73	0
3	SO4	J	301	5/5	0.96	0.13	57,58,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	H	301	5/5	0.96	0.17	54,56,59,61	0
3	SO4	A	901	5/5	0.97	0.12	56,56,59,63	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.