



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 PM GMT

PDB ID : 4LJB
Title : Structure of a photobleached state of IrisFP under high intensity laser-light
Authors : Duan, C.; Adam, V.; Byrdin, M.; Ridard, J.; Kieffer-Jacquiod, S.; Morlot, C.; Arcizet, D.; Demachy, I.; Bourgeois, D.
Deposited on : 2013-07-04
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

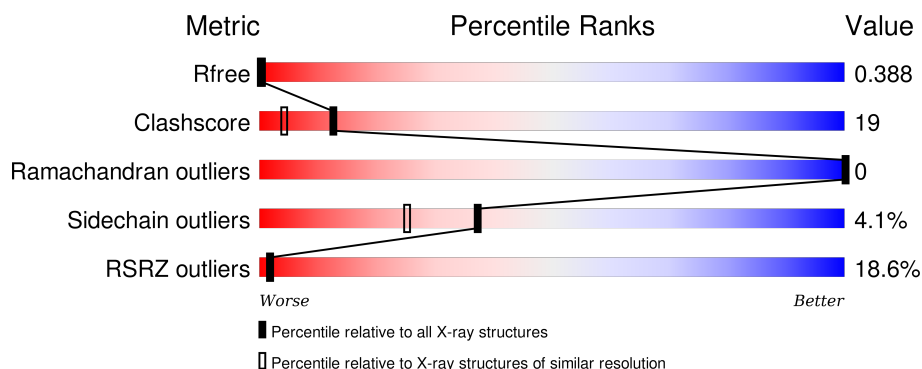
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	227	<div> <div>10%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
1	B	227	<div> <div>28%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	C	227	<div> <div>15%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	D	227	<div> <div>20%</div> <div>67%</div> <div>28%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	301	-	-	-	X
2	SO4	A	305	-	-	-	X
2	SO4	B	301	-	-	-	X
2	SO4	B	302	-	-	X	X
2	SO4	B	303	-	-	X	-
2	SO4	C	303	-	-	-	X
3	SO3	A	304	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7520 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 Green to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1778	1133	305	329	11			
1	B	220	Total	C	N	O	S	0	0	0
			1767	1127	304	326	10			
1	C	223	Total	C	N	O	S	0	1	0
			1807	1150	313	333	11			
1	D	221	Total	C	N	O	S	0	0	0
			1778	1133	305	329	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
A	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
A	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
B	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
B	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9

Continued on next page...

Continued from previous page...

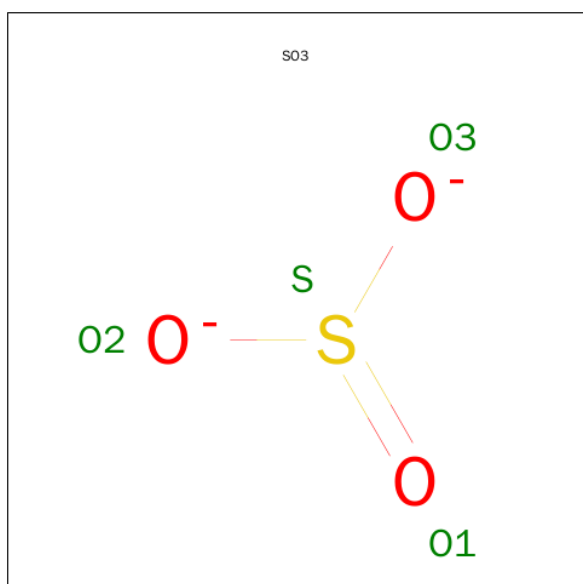
Chain	Residue	Modelled	Actual	Comment	Reference
B	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
C	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
C	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
C	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
D	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
D	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is SULFITE ION (three-letter code: SO₃) (formula: O₃S).



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

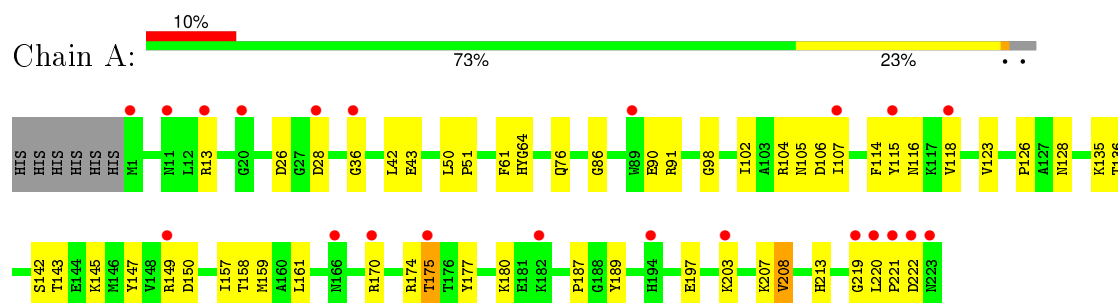
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	B	72	Total O 72 72	0	0
4	C	68	Total O 68 68	0	0
4	D	68	Total O 68 68	0	0

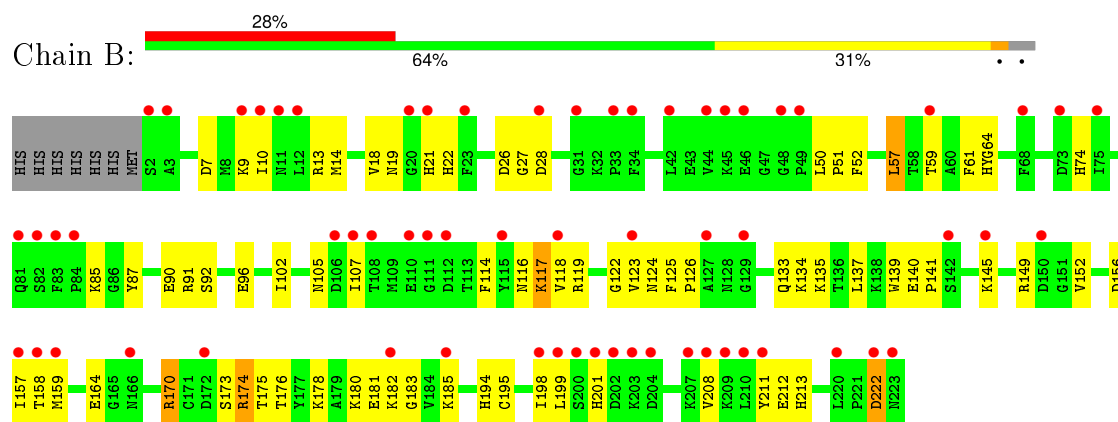
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

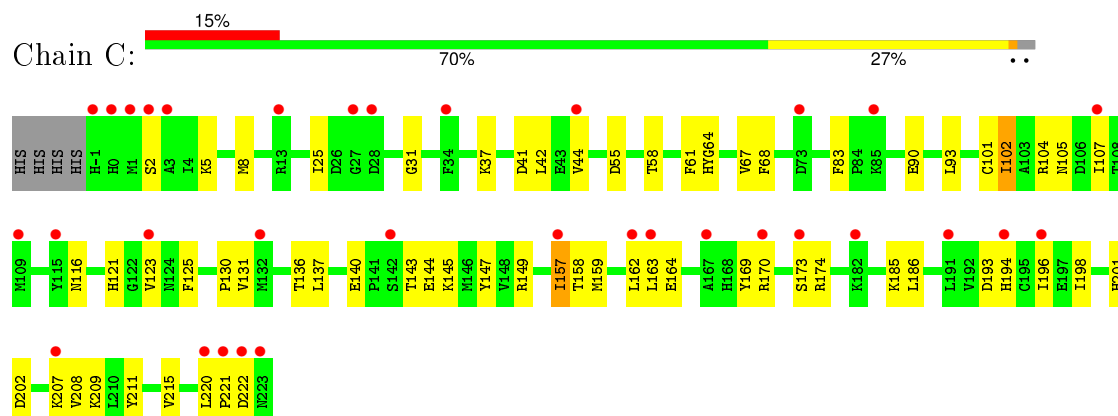
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



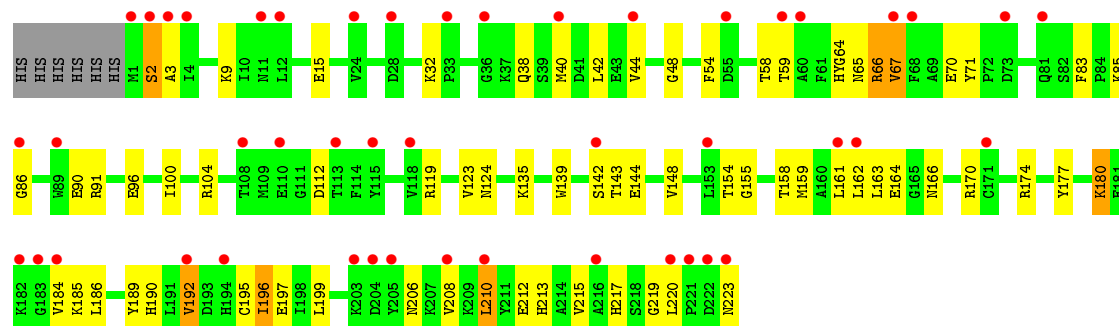
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



- Chain D:  20% 67% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.10Å 96.42Å 140.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.01 – 1.90 10.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.9 (10.01-1.90) 85.9 (10.01-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.339 , 0.384 0.346 , 0.388	Depositor DCC
R_{free} test set	3938 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	1.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtriage
Outliers	8 of 78459 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7520	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CR8, SO3, 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	0.47	0/1798	0.67	0/2424
1	B	0.44	0/1787	0.63	0/2410
1	C	0.43	0/1829	0.64	0/2466
1	D	0.48	1/1798 (0.1%)	0.65	0/2424
All	All	0.46	1/7212 (0.0%)	0.65	0/9724

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	SER	C-N	-5.34	1.21	1.34

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	1778	0	1713	54	0
1	B	1767	0	1699	97	0
1	C	1807	0	1734	61	0
1	D	1778	0	1713	94	0
2	A	20	0	0	2	0
2	B	15	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	0	0	0
2	D	10	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	105	0	0	5	0
4	B	72	0	0	5	0
4	C	68	0	0	4	0
4	D	68	0	0	14	0
All	All	7520	0	6859	273	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (273) 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:210:LEU:H	1:D:210:LEU:HD12	1.07	1.17
1:B:174:ARG:HH21	1:B:174:ARG:CG	1.66	1.08
1:A:158:THR:O	1:B:145:LYS:HE3	1.52	1.07
1:D:139:TRP:CE2	1:D:161:LEU:HD21	1.92	1.05
1:B:170:ARG:HH21	1:B:170:ARG:CG	1.68	1.04
1:B:170:ARG:HH21	1:B:170:ARG:HG3	0.82	0.97
1:B:174:ARG:HG3	1:B:174:ARG:NH2	1.52	0.97
1:D:139:TRP:CD2	1:D:161:LEU:HD21	2.00	0.97
1:D:210:LEU:HD12	1:D:210:LEU:N	1.80	0.96
1:D:219:GLY:HA2	1:D:223:ASN:HD21	1.31	0.94
1:D:42:LEU:HD11	1:D:210:LEU:HD21	1.49	0.94
1:B:170:ARG:HG3	1:B:170:ARG:NH2	1.63	0.94
1:D:40:MET:HG3	1:D:210:LEU:HD13	1.50	0.93
1:B:85:LYS:HD2	1:B:181:GLU:HB2	1.52	0.92
1:A:107:ILE:HD11	1:A:114:PHE:HB3	1.50	0.91
1:D:40:MET:O	1:D:210:LEU:HD12	1.74	0.87
1:D:42:LEU:HG	1:D:210:LEU:HD11	1.54	0.87
1:B:158:THR:O	1:B:158:THR:HG23	1.75	0.86
1:D:66:ARG:HH22	1:D:192:VAL:HG21	1.40	0.86
1:B:174:ARG:HG3	1:B:174:ARG:HH21	0.74	0.84
1:D:139:TRP:CD2	1:D:161:LEU:CD2	2.60	0.83
1:C:41:ASP:HB3	1:C:207:LYS:NZ	1.94	0.81
1:D:64:CR8:H4	4:D:415:HOH:O	1.81	0.79
1:A:107:ILE:HG13	1:A:115:TYR:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:CR8:H6	1:C:196:ILE:HD11	1.65	0.78
1:B:157:ILE:CG2	1:B:173:SER:OG	2.32	0.77
1:B:140:GLU:HG3	1:B:141:PRO:HD2	1.66	0.76
1:B:123:VAL:HG13	1:D:90:GLU:HB3	1.67	0.76
1:B:10:ILE:HG22	1:B:114:PHE:HB2	1.68	0.76
1:C:220:LEU:HG	1:C:221:PRO:HA	1.68	0.75
1:D:2:SER:HA	4:D:442:HOH:O	1.84	0.75
1:D:210:LEU:CD1	1:D:210:LEU:H	1.94	0.75
1:B:64:CR8:H23	1:B:212:GLU:HB2	1.68	0.74
1:B:183:GLY:N	2:B:303:SO4:O3	2.20	0.74
1:C:207:LYS:HD2	1:C:208:VAL:N	2.03	0.74
1:D:40:MET:HG2	1:D:64:CR8:C10	2.18	0.74
1:C:174:ARG:HH12	1:D:170:ARG:HH21	1.34	0.73
1:D:40:MET:HG2	1:D:64:CR8:H10	1.70	0.73
2:B:302:SO4:O4	1:D:104:ARG:NH1	2.22	0.73
1:C:42:LEU:O	1:C:207:LYS:HD3	1.89	0.73
1:B:22:HIS:ND1	2:B:302:SO4:O2	2.22	0.72
1:C:220:LEU:CG	1:C:221:PRO:HA	2.19	0.72
1:C:41:ASP:HB3	1:C:207:LYS:HZ1	1.53	0.72
1:D:40:MET:O	1:D:210:LEU:CD1	2.39	0.71
1:D:2:SER:CA	4:D:442:HOH:O	2.38	0.71
1:B:14:MET:HA	1:B:118:VAL:HG13	1.72	0.71
1:B:152:VAL:HG11	1:B:176:THR:HG23	1.73	0.70
1:D:40:MET:HG3	1:D:210:LEU:CD1	2.21	0.70
1:D:220:LEU:HD12	1:D:223:ASN:OD1	1.90	0.70
1:D:219:GLY:HA2	1:D:223:ASN:ND2	2.06	0.70
1:C:221:PRO:HD3	1:D:195:CYS:SG	2.33	0.68
1:B:157:ILE:HG23	1:B:173:SER:OG	1.94	0.68
1:D:219:GLY:CA	1:D:223:ASN:HD21	2.05	0.67
2:A:301:SO4:O4	1:C:104:ARG:NH1	2.27	0.67
1:A:158:THR:O	1:B:145:LYS:CE	2.37	0.67
1:D:71:TYR:CE2	4:D:449:HOH:O	2.47	0.67
1:A:170:ARG:NE	1:B:156:ASP:OD2	2.24	0.67
1:D:139:TRP:CZ3	1:D:161:LEU:HG	2.30	0.66
1:B:157:ILE:HD12	1:B:194:HIS:CE1	2.30	0.66
1:B:91:ARG:HD3	1:B:175:THR:OG1	1.95	0.66
1:D:217:HIS:ND1	1:D:223:ASN:ND2	2.44	0.66
1:B:90:GLU:HB3	1:D:123:VAL:HG13	1.78	0.64
1:B:27:GLY:O	1:B:28:ASP:OD1	2.16	0.64
1:D:219:GLY:CA	1:D:223:ASN:ND2	2.60	0.64
1:C:41:ASP:C	1:C:207:LYS:HZ2	2.01	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:THR:O	1:B:158:THR:CG2	2.46	0.64
1:B:158:THR:HA	1:B:170:ARG:HH12	1.63	0.63
1:B:157:ILE:HG22	1:B:173:SER:OG	1.98	0.63
1:C:105:ASN:ND2	1:C:107:ILE:HD11	2.13	0.63
1:D:91:ARG:NH1	4:D:415:HOH:O	2.31	0.63
1:D:42:LEU:HD12	1:D:54:PHE:HZ	1.64	0.63
1:D:42:LEU:CD1	1:D:210:LEU:HD21	2.25	0.62
1:B:198:ILE:HG23	1:B:208:VAL:HG13	1.81	0.62
1:B:182:LYS:HA	2:B:303:SO4:O3	1.99	0.62
1:B:198:ILE:HG23	1:B:208:VAL:CG1	2.30	0.61
1:D:185:LYS:HG2	1:D:186:LEU:N	2.16	0.61
1:C:174:ARG:HH12	1:D:170:ARG:NH2	1.98	0.61
1:B:105:ASN:HA	1:B:117:LYS:O	2.01	0.61
1:B:64:CR8:H23	1:B:212:GLU:CB	2.30	0.61
1:A:91:ARG:HG3	1:A:175:THR:HG22	1.82	0.61
1:D:139:TRP:CE3	1:D:161:LEU:HG	2.36	0.60
1:A:157:ILE:HG12	1:A:159:MET:HG3	1.82	0.60
1:C:220:LEU:HG	1:C:221:PRO:CA	2.30	0.60
1:C:220:LEU:CD1	1:C:221:PRO:HA	2.32	0.60
1:D:190:HIS:CE1	4:D:449:HOH:O	2.54	0.60
1:D:64:CR8:N	1:D:64:CR8:H171	2.17	0.59
1:A:142:SER:HA	1:B:145:LYS:HZ2	1.67	0.59
1:C:157:ILE:HG23	1:C:173:SER:HB3	1.84	0.59
1:B:222:ASP:N	1:B:222:ASP:OD1	2.36	0.58
1:C:220:LEU:HD12	1:C:221:PRO:HA	1.85	0.58
1:A:143:THR:H	1:B:145:LYS:HZ1	1.50	0.58
1:D:135:LYS:HE2	1:D:164:GLU:HB3	1.86	0.58
1:A:189:TYR:CD1	1:B:140:GLU:HG2	2.39	0.57
1:D:32:LYS:HD3	4:D:436:HOH:O	2.04	0.57
1:B:92:SER:CB	1:D:100:ILE:HD12	2.34	0.57
1:C:42:LEU:O	1:C:207:LYS:CD	2.53	0.57
1:C:5:LYS:O	1:C:8:MET:HG3	2.05	0.56
1:A:105:ASN:CB	1:A:118:VAL:HG22	2.34	0.56
1:A:123:VAL:HG22	1:C:102:ILE:HG13	1.87	0.56
1:C:55:ASP:OD1	1:C:198:ILE:HD11	2.05	0.56
1:B:185:LYS:HA	4:B:459:HOH:O	2.04	0.56
1:D:40:MET:CG	1:D:210:LEU:HD13	2.29	0.56
1:A:105:ASN:HB2	1:A:118:VAL:HG22	1.88	0.56
1:A:150:ASP:N	2:A:305:SO4:O4	2.29	0.56
1:C:61:PHE:C	1:C:64:CR8:H171	2.26	0.56
1:A:13:ARG:CD	1:A:26:ASP:OD1	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG13	1:D:206:ASN:HA	1.87	0.55
1:C:130:PRO:HD2	4:C:409:HOH:O	2.05	0.55
1:B:157:ILE:CG2	1:B:173:SER:HG	2.19	0.55
1:B:92:SER:OG	1:D:100:ILE:HD12	2.07	0.55
1:D:174:ARG:NH2	4:D:455:HOH:O	2.25	0.55
1:D:9:LYS:NZ	4:D:459:HOH:O	2.32	0.55
1:C:64:CR8:C6	1:C:196:ILE:HD11	2.36	0.54
1:A:135:LYS:NZ	4:A:427:HOH:O	2.20	0.54
1:B:85:LYS:HB3	1:B:180:LYS:HE2	1.89	0.54
1:A:13:ARG:HD2	1:A:26:ASP:OD1	2.07	0.54
1:B:170:ARG:CG	1:B:170:ARG:NH2	2.40	0.54
1:D:112:ASP:HB3	4:D:459:HOH:O	2.06	0.54
1:B:157:ILE:HG22	1:B:173:SER:HG	1.72	0.54
1:B:14:MET:CB	1:B:118:VAL:HG13	2.37	0.54
1:C:185:LYS:HD2	1:C:186:LEU:H	1.73	0.54
1:A:143:THR:H	1:B:145:LYS:NZ	2.05	0.54
1:A:189:TYR:CG	1:B:140:GLU:HG2	2.43	0.54
1:D:2:SER:O	1:D:3:ALA:HB3	2.07	0.54
1:D:185:LYS:HG2	1:D:186:LEU:H	1.70	0.54
1:A:145:LYS:HD3	1:B:158:THR:O	2.09	0.52
1:C:41:ASP:CA	1:C:207:LYS:HZ2	2.22	0.52
1:B:14:MET:CA	1:B:118:VAL:HG13	2.37	0.52
1:A:220:LEU:HA	1:A:221:PRO:C	2.29	0.52
1:D:70:GLU:HB3	1:D:215:VAL:HG23	1.92	0.52
1:B:133:GLN:HB3	1:B:135:LYS:HZ3	1.75	0.52
1:D:66:ARG:HD2	1:D:177:TYR:OH	2.10	0.52
1:D:42:LEU:HD12	1:D:54:PHE:CZ	2.44	0.51
1:B:158:THR:OG1	1:B:170:ARG:NH1	2.44	0.51
1:A:90:GLU:CD	4:A:419:HOH:O	2.48	0.51
1:A:135:LYS:NZ	4:A:484:HOH:O	2.43	0.51
1:A:86:GLY:C	1:A:180:LYS:HG2	2.31	0.51
1:B:117:LYS:NZ	1:B:119:ARG:HH22	2.09	0.50
1:B:135:LYS:O	1:B:164:GLU:HG3	2.12	0.50
1:B:9:LYS:O	1:B:10:ILE:HG23	2.12	0.50
1:B:14:MET:HB2	1:B:118:VAL:CG1	2.41	0.50
1:C:2:SER:N	4:C:446:HOH:O	2.45	0.50
1:C:42:LEU:N	1:C:207:LYS:HZ2	2.09	0.50
1:B:50:LEU:HD22	1:B:52:PHE:CE1	2.47	0.50
1:B:50:LEU:O	1:B:134:LYS:NZ	2.33	0.50
1:B:18:VAL:HG22	1:B:122:GLY:HA3	1.94	0.50
1:A:147:TYR:HE2	1:A:149:ARG:HD3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD12	1:A:208:VAL:HG22	1.93	0.49
1:A:107:ILE:HD12	1:A:116:ASN:OD1	2.12	0.49
1:C:93:LEU:HB2	1:C:101:CYS:HB2	1.95	0.49
1:D:139:TRP:CD2	1:D:161:LEU:HD23	2.47	0.49
1:C:185:LYS:HD2	1:C:186:LEU:N	2.28	0.49
1:C:170:ARG:HD3	4:C:460:HOH:O	2.11	0.49
1:D:197:GLU:HG2	1:D:199:LEU:HD23	1.95	0.49
1:B:59:THR:O	1:B:91:ARG:NH2	2.45	0.48
1:C:37:LYS:HE3	1:C:211:TYR:OH	2.14	0.48
1:D:64:CR8:H8	1:D:66:ARG:HH11	1.78	0.48
1:C:41:ASP:CB	1:C:207:LYS:NZ	2.73	0.48
1:B:61:PHE:O	1:B:64:CR8:H171	2.13	0.48
1:C:130:PRO:HB3	1:C:163:LEU:HD22	1.94	0.48
1:C:220:LEU:HA	1:C:222:ASP:H	1.78	0.48
1:B:13:ARG:NE	1:B:26:ASP:OD1	2.46	0.48
1:A:43:GLU:HG3	1:A:207:LYS:HE2	1.96	0.48
1:D:64:CR8:H8	1:D:66:ARG:HE	1.78	0.48
1:C:207:LYS:HD2	1:C:208:VAL:H	1.76	0.48
1:C:162:LEU:HD23	1:C:163:LEU:N	2.29	0.48
1:D:139:TRP:CE3	1:D:161:LEU:CD2	2.97	0.48
1:A:189:TYR:CD1	1:B:140:GLU:CG	2.96	0.48
1:B:14:MET:HB2	1:B:118:VAL:HG13	1.95	0.47
1:A:189:TYR:CE1	1:B:140:GLU:CG	2.97	0.47
1:D:195:CYS:SG	1:D:213:HIS:HB3	2.54	0.47
1:C:157:ILE:HG13	1:C:158:THR:N	2.30	0.47
1:B:14:MET:SD	1:B:57:LEU:HD23	2.54	0.47
1:A:105:ASN:CG	1:A:118:VAL:HG22	2.35	0.47
1:D:66:ARG:NH2	1:D:192:VAL:HG21	2.20	0.47
1:D:42:LEU:N	1:D:208:VAL:O	2.37	0.47
1:B:22:HIS:CG	2:B:302:SO4:O2	2.67	0.47
1:B:178:LYS:NZ	4:B:406:HOH:O	2.30	0.47
1:D:220:LEU:CD1	1:D:223:ASN:OD1	2.61	0.47
1:C:221:PRO:HG3	1:D:213:HIS:ND1	2.30	0.47
1:D:112:ASP:HB2	4:D:429:HOH:O	2.15	0.47
1:A:76:GLN:HB3	1:A:187:PRO:HA	1.96	0.46
1:D:144:GLU:OE2	1:D:155:GLY:HA3	2.15	0.46
1:D:64:CR8:H2	1:D:196:ILE:CD1	2.45	0.46
1:D:135:LYS:HG2	1:D:164:GLU:HB3	1.97	0.46
1:C:58:THR:HA	1:C:61:PHE:HD2	1.80	0.46
1:D:71:TYR:HE2	4:D:449:HOH:O	1.89	0.46
1:B:157:ILE:HG12	1:B:158:THR:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HB3	1:B:117:LYS:HE3	1.65	0.46
1:D:112:ASP:N	4:D:429:HOH:O	2.47	0.46
1:A:86:GLY:O	1:A:180:LYS:HG2	2.16	0.46
1:A:170:ARG:HD2	1:B:149:ARG:NH2	2.30	0.46
1:D:65:ASN:OD1	1:D:67:VAL:HG22	2.16	0.46
1:A:61:PHE:C	1:A:64:CR8:H171	2.35	0.46
1:B:152:VAL:CG1	1:B:176:THR:HG23	2.45	0.46
1:B:52:PHE:C	1:B:134:LYS:HZ3	2.18	0.45
1:D:66:ARG:HD2	1:D:177:TYR:CZ	2.51	0.45
1:C:222:ASP:O	1:C:222:ASP:OD1	2.34	0.45
1:C:125:PHE:CE1	1:C:131:VAL:HG21	2.51	0.45
1:C:31:GLY:HA3	1:C:68:PHE:CE2	2.51	0.45
1:B:157:ILE:HD12	1:B:194:HIS:HE1	1.76	0.45
1:A:149:ARG:NH2	1:B:96:GLU:OE1	2.49	0.45
1:A:123:VAL:HB	1:C:90:GLU:HB3	1.98	0.45
1:D:48:GLY:HA3	1:D:206:ASN:HD21	1.81	0.45
1:C:163:LEU:HD11	1:C:169:TYR:HB2	1.99	0.45
1:B:21:HIS:CG	1:B:51:PRO:HG3	2.52	0.45
1:B:74:HIS:O	4:B:453:HOH:O	2.21	0.45
1:B:9:LYS:O	1:B:10:ILE:CG2	2.65	0.45
1:A:219:GLY:O	1:A:222:ASP:O	2.34	0.45
1:C:157:ILE:CG2	1:C:173:SER:HB3	2.47	0.45
1:C:201:HIS:ND1	1:C:202:ASP:O	2.38	0.45
1:D:210:LEU:CD1	1:D:210:LEU:N	2.54	0.45
1:C:67:VAL:HG21	1:C:83:PHE:CE1	2.52	0.45
1:B:87:TYR:CZ	1:B:107:ILE:HD13	2.52	0.44
1:C:25:ILE:HG12	1:C:44:VAL:HG22	1.99	0.44
1:B:14:MET:HA	1:B:118:VAL:CG1	2.45	0.44
1:A:98:GLY:HA3	4:A:487:HOH:O	2.18	0.44
1:D:83:PHE:CE1	1:D:86:GLY:HA2	2.53	0.44
1:D:59:THR:HG22	1:D:64:CR8:C2	2.48	0.44
1:C:157:ILE:HG12	1:C:159:MET:HG3	2.00	0.44
1:B:137:LEU:HD21	1:B:164:GLU:HG2	2.00	0.44
1:B:157:ILE:CD1	1:B:194:HIS:CE1	3.00	0.44
1:D:85:LYS:HB3	1:D:180:LYS:HG2	2.00	0.44
1:A:149:ARG:HD2	1:A:149:ARG:HA	1.79	0.44
1:D:139:TRP:CH2	1:D:161:LEU:HD11	2.53	0.43
1:A:189:TYR:CE1	1:B:140:GLU:HG2	2.53	0.43
1:B:102:ILE:HB	1:D:123:VAL:HG21	1.99	0.43
1:D:162:LEU:HD11	1:D:166:ASN:HA	2.00	0.43
1:A:142:SER:HB2	1:B:145:LYS:HZ1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:NH1	4:A:495:HOH:O	2.33	0.43
1:D:66:ARG:HG2	4:D:425:HOH:O	2.17	0.43
1:A:189:TYR:CE1	1:B:140:GLU:HG3	2.53	0.43
1:C:136:THR:O	1:C:137:LEU:HD23	2.19	0.43
1:A:197:GLU:HB2	3:A:304:SO3:S	2.58	0.43
1:C:58:THR:HA	1:C:61:PHE:CD2	2.53	0.43
1:D:96:GLU:OE2	1:D:170:ARG:N	2.45	0.43
1:D:158:THR:HG23	1:D:158:THR:O	2.19	0.43
1:B:117:LYS:HZ1	1:B:119:ARG:HH22	1.67	0.43
1:B:125:PHE:HA	1:B:126:PRO:HD3	1.87	0.43
1:D:104:ARG:NH1	1:D:119:ARG:HG3	2.34	0.42
1:C:145:LYS:NZ	1:D:159:MET:HA	2.34	0.42
1:D:38:GLN:HG3	1:D:212:GLU:CG	2.49	0.42
1:D:139:TRP:CG	1:D:161:LEU:CD2	3.02	0.42
1:B:158:THR:CA	1:B:170:ARG:HH12	2.32	0.42
1:D:123:VAL:HG12	1:D:124:ASN:CG	2.40	0.42
1:A:136:THR:HG21	1:A:161:LEU:HD13	2.01	0.42
1:A:104:ARG:NH1	1:A:106:ASP:OD1	2.49	0.42
1:C:145:LYS:HZ3	1:D:142:SER:HB2	1.84	0.42
1:B:139:TRP:N	4:B:401:HOH:O	2.21	0.42
1:C:147:TYR:OH	1:C:149:ARG:NH2	2.42	0.42
1:C:144:GLU:HB2	1:C:194:HIS:HE1	1.85	0.42
1:D:135:LYS:HD3	1:D:163:LEU:HB3	2.02	0.42
1:A:64:CR8:N	1:A:64:CR8:H171	2.35	0.42
1:C:143:THR:HG22	1:C:193:ASP:OD1	2.18	0.42
1:D:208:VAL:HG12	1:D:210:LEU:HG	2.00	0.41
1:C:170:ARG:CD	4:C:460:HOH:O	2.68	0.41
1:A:102:ILE:HD11	1:C:121:HIS:HB3	2.01	0.41
1:B:211:TYR:OH	1:B:213:HIS:HB2	2.21	0.41
1:A:36:GLY:O	1:A:213:HIS:HA	2.19	0.41
1:B:123:VAL:CG1	1:D:90:GLU:HB3	2.45	0.41
1:A:189:TYR:CD2	1:B:140:GLU:HG2	2.56	0.41
1:D:142:SER:OG	1:D:143:THR:N	2.51	0.41
1:A:175:THR:OG1	1:A:177:TYR:CE2	2.74	0.41
1:B:199:LEU:HD11	1:B:211:TYR:HB2	2.02	0.41
1:C:140:GLU:HB3	1:D:189:TYR:CE2	2.56	0.41
1:B:122:GLY:O	4:B:454:HOH:O	2.22	0.41
1:B:201:HIS:CB	1:B:208:VAL:HG22	2.52	0.40
1:B:64:CR8:H5	1:B:91:ARG:NH1	2.36	0.40
1:C:137:LEU:HD21	1:C:164:GLU:HG2	2.04	0.40
1:A:50:LEU:HA	1:A:51:PRO:HD3	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:HIS:HB2	1:B:208:VAL:HG22	2.03	0.40
1:D:154:THR:HG21	1:D:174:ARG:HE	1.86	0.40
1:A:126:PRO:HB2	1:A:128:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

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	218/227 (96%)	216 (99%)	2 (1%)	0	100	100
1	B	217/227 (96%)	215 (99%)	2 (1%)	0	100	100
1	C	221/227 (97%)	215 (97%)	6 (3%)	0	100	100
1	D	218/227 (96%)	216 (99%)	2 (1%)	0	100	100
All	All	874/908 (96%)	862 (99%)	12 (1%)	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	188/195 (96%)	184 (98%)	4 (2%)	61	55
1	B	186/195 (95%)	175 (94%)	11 (6%)	24	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	191/195 (98%)	185 (97%)	6 (3%)	47	37
1	D	188/195 (96%)	178 (95%)	10 (5%)	28	16
All	All	753/780 (96%)	722 (96%)	31 (4%)	37	25

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	175	THR
1	A	203	LYS
1	A	208	VAL
1	B	7	ASP
1	B	19	ASN
1	B	57	LEU
1	B	116	ASN
1	B	117	LYS
1	B	124	ASN
1	B	159	MET
1	B	170	ARG
1	B	174	ARG
1	B	195	CYS
1	B	222	ASP
1	C	102	ILE
1	C	116	ASN
1	C	123	VAL
1	C	157	ILE
1	C	209	LYS
1	C	215	VAL
1	D	15	GLU
1	D	58	THR
1	D	66	ARG
1	D	67	VAL
1	D	148	VAL
1	D	180	LYS
1	D	184	VAL
1	D	192	VAL
1	D	196	ILE
1	D	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	B	124	ASN
1	D	22	HIS
1	D	223	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	CR8	A	64	1	20,27,28	1.81	7 (35%)	16,37,39	1.12	2 (12%)
1	CR8	B	64	1	20,27,28	1.70	5 (25%)	16,37,39	1.64	4 (25%)
1	CR8	C	64	1	20,27,28	1.85	4 (20%)	16,37,39	0.99	1 (6%)
1	CR8	D	64	1	20,27,28	1.74	5 (25%)	16,37,39	1.92	5 (31%)

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
1	CR8	A	64	1	-	0/8/25/26	0/3/3/3
1	CR8	B	64	1	-	0/8/25/26	0/3/3/3
1	CR8	C	64	1	-	0/8/25/26	0/3/3/3
1	CR8	D	64	1	-	1/8/25/26	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	CR8	C2-C1	-3.37	1.38	1.45
1	C	64	CR8	C2-C1	-2.90	1.39	1.45
1	C	64	CR8	C4-C1	-2.86	1.39	1.45
1	A	64	CR8	C2-C1	-2.72	1.39	1.45
1	B	64	CR8	C4-C1	-2.70	1.39	1.45
1	B	64	CR8	C2-C1	-2.54	1.40	1.45
1	D	64	CR8	C4-C1	-2.49	1.40	1.45
1	A	64	CR8	C4-C1	-2.39	1.40	1.45
1	A	64	CR8	C6-C2	2.01	1.40	1.35
1	B	64	CR8	C14-N15	2.06	1.38	1.34
1	A	64	CR8	C5-C4	2.09	1.40	1.35
1	D	64	CR8	C14-N15	2.13	1.38	1.34
1	B	64	CR8	C9-C8	2.23	1.48	1.40
1	A	64	CR8	C9-C8	2.28	1.49	1.40
1	D	64	CR8	C9-C8	2.32	1.49	1.40
1	A	64	CR8	C14-N15	2.33	1.39	1.34
1	C	64	CR8	C9-C8	2.44	1.49	1.40
1	D	64	CR8	C8-C7	4.46	1.47	1.36
1	B	64	CR8	C8-C7	4.67	1.47	1.36
1	A	64	CR8	C8-C7	5.15	1.49	1.36
1	C	64	CR8	C8-C7	5.29	1.49	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	C4-C5-C7	-4.50	118.01	122.00
1	B	64	CR8	C2-C6-C7	-3.89	118.55	122.00
1	D	64	CR8	C-C17-N13	-3.11	107.32	112.37
1	D	64	CR8	O3-C1-C2	-2.95	116.86	121.51
1	D	64	CR8	C6-C7-C8	-2.33	115.29	121.85
1	C	64	CR8	C2-C6-C7	-2.28	119.97	122.00
1	A	64	CR8	C4-C5-C7	-2.11	120.13	122.00
1	B	64	CR8	C5-C7-C8	-2.09	115.97	121.85
1	A	64	CR8	C23-N11-C10	2.04	108.93	105.71
1	B	64	CR8	C16-C14-N15	2.11	128.43	123.77
1	B	64	CR8	C6-C7-C5	2.17	120.86	116.13
1	D	64	CR8	C6-C7-C5	2.21	120.95	116.13

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	64	CR8	C7-C8-C9-N15

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	64	CR8	2	0
1	B	64	CR8	4	0
1	C	64	CR8	3	0
1	D	64	CR8	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	301	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	302	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO3	A	304	-	1,3,3	0.81	0	0,3,3	0.00	-
2	SO4	A	305	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	B	301	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	302	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	B	303	-	4,4,4	1.14	1 (25%)	6,6,6	0.31	0
3	SO3	B	304	-	1,3,3	0.62	0	0,3,3	0.00	-
2	SO4	C	301	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	C	303	-	4,4,4	0.82	0	6,6,6	0.81	0
3	SO3	C	304	-	1,3,3	0.62	0	0,3,3	0.00	-
2	SO4	C	305	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	302	-	4,4,4	0.25	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	SO3	A	304	-	-	0/0/0/0	0/0/0/0
2	SO4	A	305	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	303	-	-	0/0/0/0	0/0/0/0
3	SO3	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	SO4	C	303	-	-	0/0/0/0	0/0/0/0
3	SO3	C	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	305	-	-	0/0/0/0	0/0/0/0
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0
2	SO4	D	302	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	SO4	O4-S	-2.01	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0
3	A	304	SO3	1	0
2	A	305	SO4	1	0
2	B	302	SO4	3	0
2	B	303	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	220/227 (96%)	1.00	22 (10%) 9 10	12, 19, 33, 88	0
1	B	219/227 (96%)	1.55	63 (28%) 1 0	16, 30, 51, 72	0
1	C	222/227 (97%)	1.25	33 (14%) 3 3	12, 24, 42, 107	0
1	D	220/227 (96%)	1.56	46 (20%) 1 1	15, 26, 40, 101	0
All	All	881/908 (97%)	1.34	164 (18%) 2 2	12, 24, 46, 107	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	18.2
1	D	2	SER	13.2
1	D	222	ASP	8.0
1	B	2	SER	7.5
1	C	223	ASN	7.3
1	A	223	ASN	7.3
1	A	222	ASP	6.8
1	B	3	ALA	6.8
1	C	-1	HIS	6.5
1	C	222	ASP	6.0
1	C	0	HIS	5.8
1	C	220	LEU	5.5
1	A	221	PRO	5.2
1	C	221	PRO	5.2
1	B	10	ILE	5.0
1	D	223	ASN	4.9
1	B	207	LYS	4.9
1	C	3	ALA	4.9
1	A	1	MET	4.6
1	D	220	LEU	4.2
1	B	110	GLU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	142	SER	3.7
1	C	157	ILE	3.7
1	B	127	ALA	3.6
1	A	13	ARG	3.6
1	A	107	ILE	3.6
1	C	34	PHE	3.5
1	B	115	TYR	3.5
1	B	83	PHE	3.5
1	B	199	LEU	3.5
1	D	73	ASP	3.5
1	D	203	LYS	3.5
1	B	204	ASP	3.4
1	B	118	VAL	3.4
1	D	24	VAL	3.4
1	D	3	ALA	3.4
1	B	59	THR	3.3
1	D	4	ILE	3.3
1	D	161	LEU	3.3
1	B	158	THR	3.3
1	D	44	VAL	3.3
1	B	42	LEU	3.2
1	B	220	LEU	3.2
1	C	162	LEU	3.2
1	B	9	LYS	3.1
1	D	28	ASP	3.1
1	B	21	HIS	3.1
1	B	129	GLY	3.1
1	A	220	LEU	3.1
1	B	46	GLU	3.0
1	D	184	VAL	3.0
1	B	210	LEU	3.0
1	B	49	PRO	3.0
1	B	20	GLY	3.0
1	D	113	THR	3.0
1	D	221	PRO	3.0
1	D	192	VAL	2.9
1	A	28	ASP	2.9
1	D	171	CYS	2.9
1	A	11	ASN	2.9
1	D	11	ASN	2.9
1	B	28	ASP	2.9
1	D	86	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	67	VAL	2.8
1	D	208	VAL	2.8
1	B	108	THR	2.8
1	A	89	TRP	2.8
1	A	182	LYS	2.8
1	C	27	GLY	2.8
1	B	222	ASP	2.8
1	B	82	SER	2.8
1	C	44	VAL	2.7
1	D	118	VAL	2.7
1	D	194	HIS	2.7
1	B	211	TYR	2.7
1	C	167	ALA	2.7
1	A	203	LYS	2.7
1	B	203	LYS	2.7
1	B	209	LYS	2.6
1	A	115	TYR	2.6
1	C	142	SER	2.6
1	B	223	ASN	2.6
1	B	44	VAL	2.6
1	B	107	ILE	2.6
1	B	75	ILE	2.6
1	B	157	ILE	2.6
1	C	2	SER	2.6
1	A	166	ASN	2.6
1	C	207	LYS	2.6
1	B	166	ASN	2.5
1	B	111	GLY	2.5
1	D	183	GLY	2.5
1	A	194	HIS	2.5
1	C	1	MET	2.5
1	B	81	GLN	2.5
1	D	81	GLN	2.5
1	C	13	ARG	2.5
1	B	23	PHE	2.4
1	D	59	THR	2.4
1	B	198	ILE	2.4
1	C	107	ILE	2.4
1	C	196	ILE	2.4
1	C	132	MET	2.4
1	C	191	LEU	2.4
1	B	185	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	159	MET	2.4
1	D	40	MET	2.4
1	C	194	HIS	2.4
1	D	60	ALA	2.4
1	B	34	PHE	2.4
1	A	20	GLY	2.3
1	D	115	TYR	2.3
1	B	150	ASP	2.3
1	D	153	LEU	2.3
1	D	110	GLU	2.3
1	B	112	ASP	2.3
1	D	36	GLY	2.3
1	B	11	ASN	2.2
1	B	202	ASP	2.2
1	A	118	VAL	2.2
1	A	149	ARG	2.2
1	D	12	LEU	2.2
1	C	170	ARG	2.2
1	C	28	ASP	2.2
1	D	55	ASP	2.2
1	D	68	PHE	2.2
1	C	163	LEU	2.2
1	C	123	VAL	2.2
1	D	33	PRO	2.2
1	C	85	LYS	2.2
1	B	106	ASP	2.2
1	D	108	THR	2.2
1	B	68	PHE	2.2
1	A	170	ARG	2.1
1	D	210	LEU	2.1
1	A	175	THR	2.1
1	D	205	TYR	2.1
1	B	84	PRO	2.1
1	B	142	SER	2.1
1	D	204	ASP	2.1
1	B	45	LYS	2.1
1	B	182	LYS	2.1
1	C	109	MET	2.1
1	D	89	TRP	2.1
1	B	48	GLY	2.1
1	A	219	GLY	2.1
1	B	31	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	208	VAL	2.1
1	A	36	GLY	2.1
1	B	145	LYS	2.0
1	B	172	ASP	2.1
1	D	182	LYS	2.0
1	C	115	TYR	2.0
1	C	173	SER	2.0
1	D	162	LEU	2.0
1	B	123	VAL	2.0
1	B	201	HIS	2.0
1	C	182	LYS	2.0
1	B	200	SER	2.0
1	B	12	LEU	2.0
1	B	33	PRO	2.0
1	D	216	ALA	2.0
1	B	73	ASP	2.0
1	C	73	ASP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	C	64	25/26	0.80	0.21	-	21,30,44,47	0
1	CR8	D	64	25/26	0.71	0.29	-	21,43,54,55	0
1	CR8	A	64	25/26	0.77	0.26	-	13,26,52,59	0
1	CR8	B	64	25/26	0.65	0.33	-	39,48,59,63	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO3	A	304	4/4	0.60	0.52	19.89	11,13,16,18	4
2	SO4	C	303	5/5	0.58	0.55	10.25	22,27,27,28	5
2	SO4	A	301	5/5	0.73	0.24	4.94	81,82,82,83	0
2	SO4	A	305	5/5	0.62	0.37	2.90	93,94,95,95	0
2	SO4	B	302	5/5	0.79	0.28	2.62	97,97,97,98	0
2	SO4	B	301	5/5	0.72	0.33	2.36	78,80,80,81	0
2	SO4	D	301	5/5	0.77	0.21	1.61	86,87,87,89	0
2	SO4	C	302	5/5	0.80	0.27	-	46,47,47,48	5
2	SO4	C	301	5/5	0.76	0.31	-	99,99,100,101	0
2	SO4	D	302	5/5	0.87	0.23	-	29,36,37,38	5
2	SO4	C	305	5/5	0.46	0.37	-	86,89,90,90	0
3	SO3	C	304	4/4	0.01	0.71	-	116,118,118,118	0
3	SO3	B	304	4/4	0.80	0.41	-	36,36,36,38	4
2	SO4	A	303	5/5	0.67	0.40	-	29,30,33,36	5
2	SO4	B	303	5/5	0.74	0.28	-	47,48,49,49	5
2	SO4	A	302	5/5	0.51	0.34	-	70,70,70,71	5

6.5 Other polymers ⓘ

There are no such residues in this entry.