



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:07 pm GMT

PDB ID : 5IHL  
Title : STRUCTURE OF THE EXTRACELLULAR DOMAIN OF THE CD40 IN  
COMPLEX WITH 3H56-5 DAB  
Authors : Sheriff, S.  
Deposited on : 2016-02-29  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

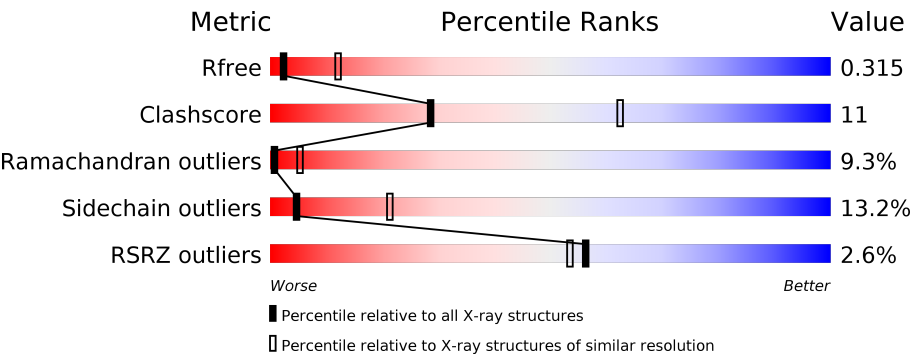
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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  $\geq 3$ , 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	183	<div><div></div><div><div></div><div>51%</div><div>30%</div><div>10%</div><div>•</div><div>8%</div></div></div>
1	D	183	<div><div>5%</div><div><div></div><div>56%</div><div>28%</div><div>5%</div><div>•</div><div>10%</div></div></div>
1	F	183	<div><div>4%</div><div><div></div><div>56%</div><div>26%</div><div>6%</div><div>•</div><div>10%</div></div></div>
1	H	183	<div><div>4%</div><div><div></div><div>57%</div><div>23%</div><div>9%</div><div>•</div><div>9%</div></div></div>
2	B	121	<div><div></div><div><div></div><div>71%</div><div>22%</div><div>•</div><div>•</div></div></div>
2	E	121	<div><div>2%</div><div><div></div><div>71%</div><div>24%</div><div>•</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	121	<div><div></div><div>74%</div><div>20%</div><div></div><div></div></div>
2	I	121	<div><div>2%</div><div></div><div>68%</div><div>28%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8291 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 Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1224	744	207	253	20			
1	D	165	Total	C	N	O	S	0	0	0
			1130	677	199	234	20			
1	F	165	Total	C	N	O	S	0	0	0
			1178	722	199	237	20			
1	H	167	Total	C	N	O	S	0	0	0
			1164	705	201	238	20			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	ASN	SEE REMARK 999	UNP P25942
A	180	ASP	ASN	SEE REMARK 999	UNP P25942
A	194	ASP	-	expression tag	UNP P25942
A	195	PRO	-	expression tag	UNP P25942
A	196	GLY	-	expression tag	UNP P25942
A	197	GLY	-	expression tag	UNP P25942
A	198	GLY	-	expression tag	UNP P25942
A	199	GLY	-	expression tag	UNP P25942
A	200	GLY	-	expression tag	UNP P25942
A	201	ARG	-	expression tag	UNP P25942
A	202	LEU	-	expression tag	UNP P25942
A	203	VAL	-	expression tag	UNP P25942
A	204	PRO	-	expression tag	UNP P25942
A	205	ARG	-	expression tag	UNP P25942
D	153	ASP	ASN	SEE REMARK 999	UNP P25942
D	180	ASP	ASN	SEE REMARK 999	UNP P25942
D	194	ASP	-	expression tag	UNP P25942
D	195	PRO	-	expression tag	UNP P25942
D	196	GLY	-	expression tag	UNP P25942
D	197	GLY	-	expression tag	UNP P25942
D	198	GLY	-	expression tag	UNP P25942

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Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLY	-	expression tag	UNP P25942
D	200	GLY	-	expression tag	UNP P25942
D	201	ARG	-	expression tag	UNP P25942
D	202	LEU	-	expression tag	UNP P25942
D	203	VAL	-	expression tag	UNP P25942
D	204	PRO	-	expression tag	UNP P25942
D	205	ARG	-	expression tag	UNP P25942
F	153	ASP	ASN	SEE REMARK 999	UNP P25942
F	180	ASP	ASN	SEE REMARK 999	UNP P25942
F	194	ASP	-	expression tag	UNP P25942
F	195	PRO	-	expression tag	UNP P25942
F	196	GLY	-	expression tag	UNP P25942
F	197	GLY	-	expression tag	UNP P25942
F	198	GLY	-	expression tag	UNP P25942
F	199	GLY	-	expression tag	UNP P25942
F	200	GLY	-	expression tag	UNP P25942
F	201	ARG	-	expression tag	UNP P25942
F	202	LEU	-	expression tag	UNP P25942
F	203	VAL	-	expression tag	UNP P25942
F	204	PRO	-	expression tag	UNP P25942
F	205	ARG	-	expression tag	UNP P25942
H	153	ASP	ASN	SEE REMARK 999	UNP P25942
H	180	ASP	ASN	SEE REMARK 999	UNP P25942
H	194	ASP	-	expression tag	UNP P25942
H	195	PRO	-	expression tag	UNP P25942
H	196	GLY	-	expression tag	UNP P25942
H	197	GLY	-	expression tag	UNP P25942
H	198	GLY	-	expression tag	UNP P25942
H	199	GLY	-	expression tag	UNP P25942
H	200	GLY	-	expression tag	UNP P25942
H	201	ARG	-	expression tag	UNP P25942
H	202	LEU	-	expression tag	UNP P25942
H	203	VAL	-	expression tag	UNP P25942
H	204	PRO	-	expression tag	UNP P25942
H	205	ARG	-	expression tag	UNP P25942

- Molecule 2 is a protein called 3H56-5 domain antibody (dAb).

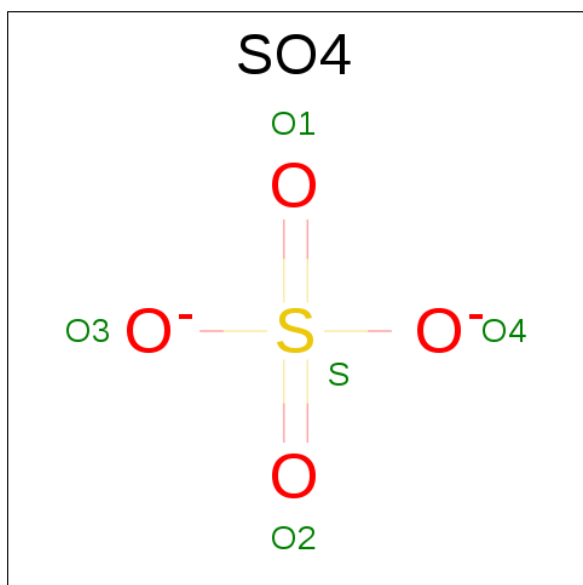
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			893	563	151	174	5			
2	E	118	Total	C	N	O	S	0	0	0
			889	562	149	173	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	117	Total	C	N	O	S	0	0	0
			895	566	152	172	5			
2	I	117	Total	C	N	O	S	0	0	0
			898	566	152	175	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

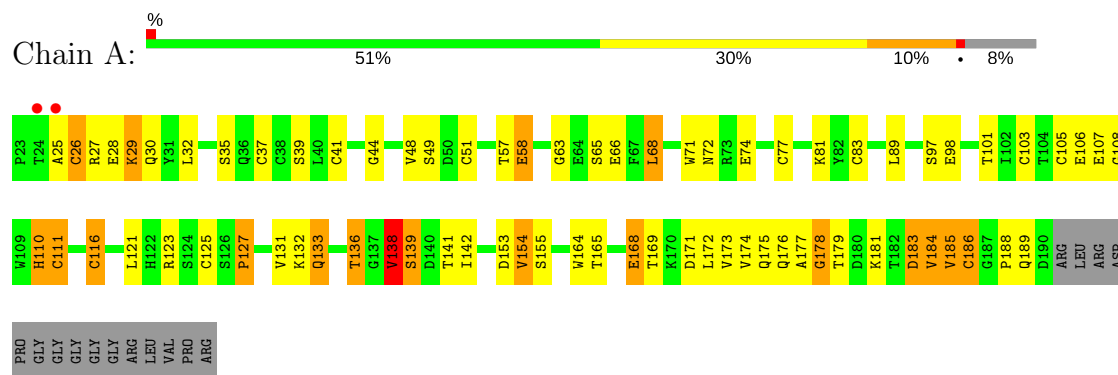


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

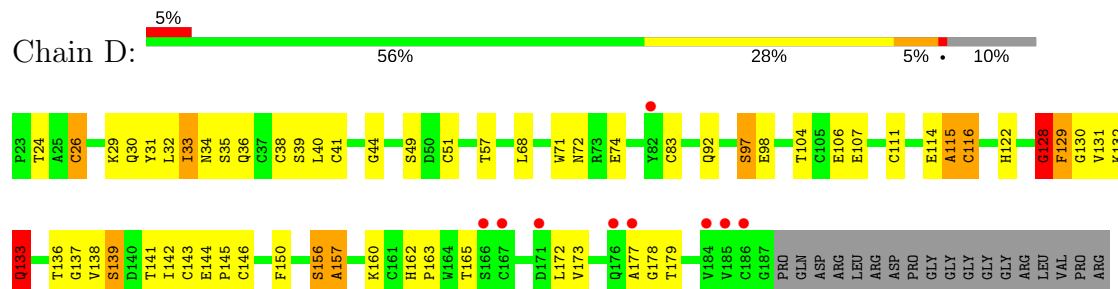
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

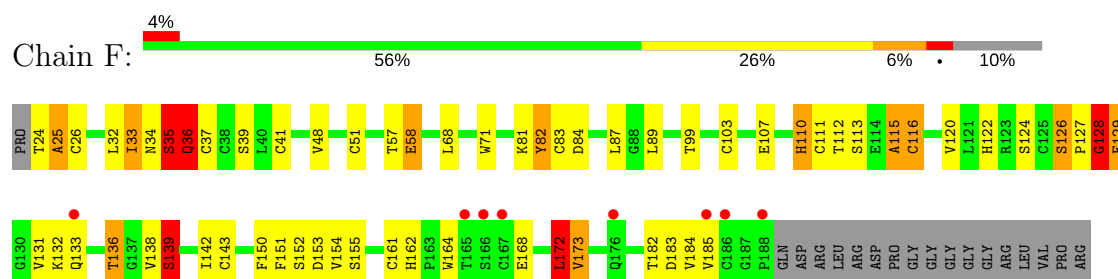
- Molecule 1: Tumor necrosis factor receptor superfamily member 5



- Molecule 1: Tumor necrosis factor receptor superfamily member 5

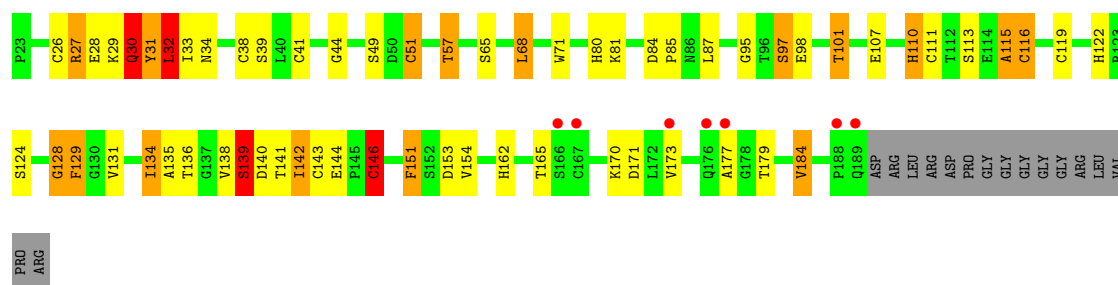


- Molecule 1: Tumor necrosis factor receptor superfamily member 5

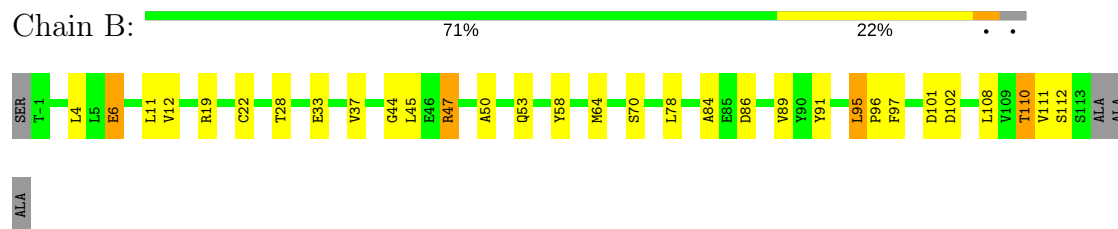


- Molecule 1: Tumor necrosis factor receptor superfamily member 5

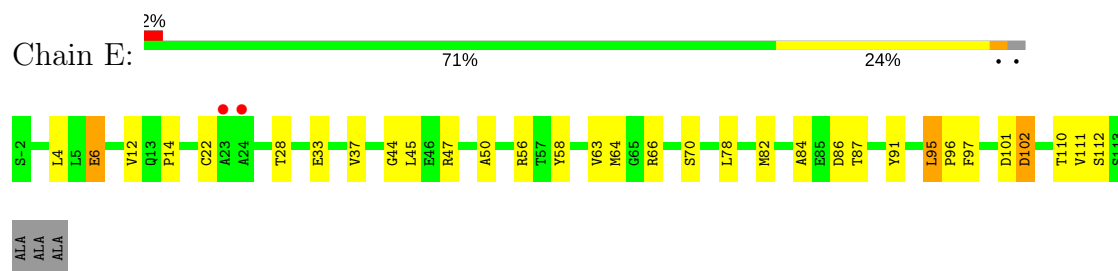




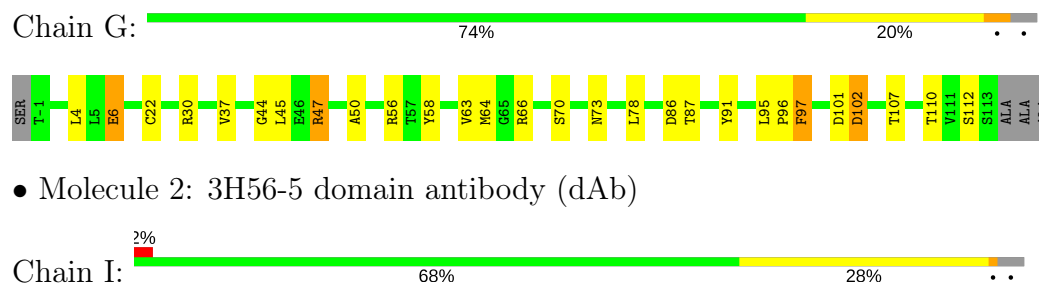
- Molecule 2: 3H56-5 domain antibody (dAb)



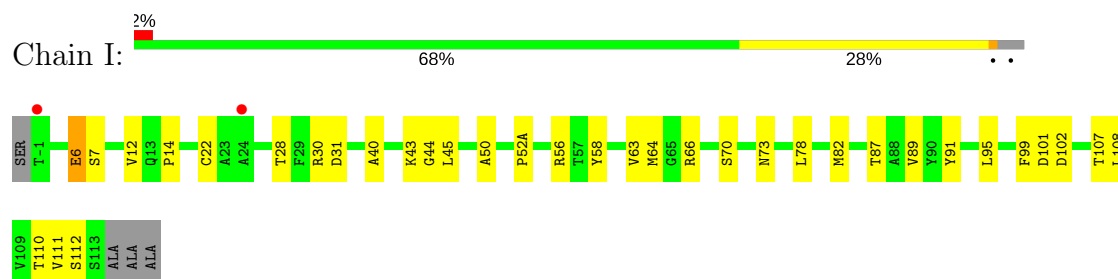
- Molecule 2: 3H56-5 domain antibody (dAb)



- Molecule 2: 3H56-5 domain antibody (dAb)



- Molecule 2: 3H56-5 domain antibody (dAb)





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.60Å 158.30Å 200.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.04 – 3.30 29.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.04-3.30) 90.8 (29.04-3.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.03 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.268 , 0.298 0.275 , 0.315	Depositor DCC
$R_{free}$ test set	953 reflections (2.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.085 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.0061e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.68	0/1252	0.97	3/1708 (0.2%)
1	D	0.53	0/1152	0.94	4/1576 (0.3%)
1	F	0.52	0/1205	0.91	4/1648 (0.2%)
1	H	0.56	0/1188	0.95	4/1622 (0.2%)
2	B	0.48	0/913	0.76	0/1242
2	E	0.44	0/909	0.73	0/1237
2	G	0.43	0/915	0.74	0/1242
2	I	0.46	0/918	0.71	0/1246
All	All	0.53	0/8452	0.86	15/11521 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	SER	C-N-CA	6.70	138.46	121.70
1	A	138	VAL	C-N-CA	6.29	137.42	121.70
1	H	128	GLY	C-N-CA	6.23	137.27	121.70
1	D	34	ASN	C-N-CA	5.97	136.63	121.70
1	D	128	GLY	C-N-CA	5.84	136.29	121.70
1	F	128	GLY	C-N-CA	5.83	136.28	121.70
1	F	34	ASN	C-N-CA	5.54	135.55	121.70
1	F	172	LEU	C-N-CA	5.38	135.14	121.70
1	D	132	LYS	C-N-CA	5.30	134.96	121.70
1	H	30	GLN	N-CA-C	-5.23	96.89	111.00
1	H	68	LEU	C-N-CA	5.19	134.68	121.70
1	F	35	SER	C-N-CA	5.17	134.62	121.70
1	A	132	LYS	C-N-CA	5.15	134.56	121.70
1	A	68	LEU	C-N-CA	5.09	134.44	121.70
1	H	32	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1224	0	1035	32	0
1	D	1130	0	891	25	0
1	F	1178	0	986	33	0
1	H	1164	0	957	32	0
2	B	893	0	833	14	0
2	E	889	0	831	18	0
2	G	895	0	844	13	0
2	I	898	0	847	15	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	G	5	0	0	0	0
All	All	8291	0	7224	170	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 11.

All (170) 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:B:84:ALA:HA	2:B:111:VAL:HG21	1.34	1.04
2:E:84:ALA:HA	2:E:111:VAL:HG21	1.54	0.90
1:F:35:SER:HA	1:F:36:GLN:O	1.82	0.80
1:F:128:GLY:HA3	1:F:129:PHE:HB2	1.68	0.76
1:D:136:THR:HA	1:D:138:VAL:N	2.00	0.76
1:F:115:ALA:HA	1:F:116:CYS:HB2	1.68	0.75
1:A:177:ALA:HB2	1:A:184:VAL:H	1.50	0.75
1:A:185:VAL:HG13	1:A:186:CYS:H	1.53	0.72
1:F:136:THR:HA	1:F:138:VAL:N	2.05	0.72
1:H:115:ALA:HA	1:H:116:CYS:HB2	1.70	0.71
2:G:6:GLU:HG2	2:G:107:THR:HG22	1.73	0.71
2:G:6:GLU:OE1	2:G:91:TYR:HA	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HA	1:A:138:VAL:N	2.07	0.69
2:E:37:VAL:HG12	2:E:47:ARG:HA	1.75	0.69
1:D:115:ALA:HA	1:D:116:CYS:HB2	1.74	0.69
2:B:6:GLU:OE1	2:B:91:TYR:HA	1.93	0.69
1:H:27:ARG:HH21	1:H:28:GLU:HB3	1.56	0.69
1:F:48:VAL:HG22	1:F:58:GLU:HB3	1.74	0.68
2:I:6:GLU:OE1	2:I:91:TYR:HA	1.92	0.68
1:F:182:THR:CB	1:F:183:ASP:HA	2.23	0.68
2:E:6:GLU:OE1	2:E:91:TYR:HA	1.93	0.68
1:H:134:ILE:HG22	1:H:135:ALA:H	1.58	0.67
2:E:12:VAL:O	2:E:111:VAL:HA	1.95	0.67
2:B:50:ALA:HB3	2:B:58:TYR:HB3	1.76	0.66
1:D:136:THR:HA	1:D:138:VAL:H	1.61	0.66
1:F:110:HIS:HB2	1:F:139:SER:O	1.96	0.66
2:E:50:ALA:HB3	2:E:58:TYR:HB3	1.78	0.66
2:G:30:ARG:HG2	2:G:73:ASN:HB3	1.78	0.65
1:A:103:CYS:HB2	1:A:116:CYS:HB3	1.79	0.65
2:B:37:VAL:HG12	2:B:47:ARG:HA	1.78	0.65
2:G:37:VAL:HG12	2:G:47:ARG:HA	1.78	0.65
1:D:150:PHE:HA	1:D:163:PRO:HA	1.79	0.65
2:B:84:ALA:HA	2:B:111:VAL:CG2	2.22	0.64
2:I:50:ALA:HB3	2:I:58:TYR:HB3	1.79	0.64
2:I:30:ARG:HG2	2:I:73:ASN:HB3	1.80	0.64
1:H:131:VAL:HG11	1:H:134:ILE:HD13	1.79	0.63
1:D:29:LYS:O	1:D:40:LEU:HD12	1.97	0.63
1:A:173:VAL:HA	1:A:186:CYS:HB3	1.80	0.63
1:A:48:VAL:HG22	1:A:58:GLU:HB3	1.80	0.62
1:D:162:HIS:CE1	2:E:56:ARG:HD2	2.35	0.62
2:E:97:PHE:O	2:E:102:ASP:HB2	1.99	0.62
1:A:165:THR:H	1:A:183:ASP:HB2	1.65	0.62
2:G:50:ALA:HB3	2:G:58:TYR:HB3	1.81	0.61
1:F:33:ILE:C	1:F:35:SER:H	2.03	0.61
2:B:111:VAL:HG23	2:B:112:SER:H	1.66	0.60
2:B:84:ALA:CA	2:B:111:VAL:HG21	2.22	0.60
2:B:111:VAL:HG23	2:B:112:SER:N	2.17	0.59
1:F:128:GLY:HA3	1:F:129:PHE:CB	2.31	0.59
1:A:172:LEU:O	1:A:186:CYS:HB2	2.02	0.58
1:H:162:HIS:NE2	2:I:56:ARG:HD2	2.18	0.58
1:F:126:SER:HB2	1:F:127:PRO:HA	1.86	0.58
1:A:108:GLY:HA2	1:A:136:THR:HG21	1.86	0.58
1:H:128:GLY:HA3	1:H:129:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HB3	1:A:30:GLN:HG3	1.86	0.57
1:H:44:GLY:HA2	1:H:97:SER:O	2.05	0.57
1:D:136:THR:HG22	1:D:139:SER:HA	1.85	0.57
2:E:84:ALA:HA	2:E:111:VAL:CG2	2.31	0.57
1:A:44:GLY:HA2	1:A:97:SER:O	2.03	0.57
1:D:44:GLY:HA2	1:D:97:SER:O	2.05	0.56
1:A:174:VAL:HG12	1:A:186:CYS:HA	1.86	0.56
2:E:95:LEU:HG	2:E:96:PRO:HA	1.88	0.56
1:F:128:GLY:CA	1:F:129:PHE:HB2	2.33	0.56
2:I:14:PRO:HD3	2:I:112:SER:O	2.05	0.56
1:H:151:PHE:CZ	1:H:153:ASP:HB2	2.42	0.55
1:F:128:GLY:HA3	1:F:129:PHE:CD2	2.41	0.55
1:H:134:ILE:HG22	1:H:135:ALA:N	2.21	0.55
1:H:80:HIS:HB3	1:H:101:THR:HG22	1.88	0.55
1:D:156:SER:HA	1:D:157:ALA:HB3	1.88	0.54
1:F:151:PHE:HB3	1:F:164:TRP:HE1	1.72	0.54
1:H:128:GLY:HA3	1:H:129:PHE:HB2	1.88	0.54
2:I:89:VAL:HG22	2:I:108:LEU:HD13	1.90	0.54
1:D:156:SER:HA	1:D:157:ALA:CB	2.38	0.54
1:H:128:GLY:HA3	1:H:129:PHE:HD2	1.71	0.54
2:I:6:GLU:HB3	2:I:107:THR:HB	1.89	0.53
1:A:164:TRP:HZ2	1:A:178:GLY:HA2	1.74	0.53
1:A:185:VAL:HG13	1:A:186:CYS:N	2.23	0.53
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.90	0.53
2:I:6:GLU:HG2	2:I:107:THR:HG22	1.90	0.53
1:F:136:THR:HA	1:F:138:VAL:H	1.74	0.53
1:A:136:THR:C	1:A:138:VAL:H	2.13	0.52
2:E:14:PRO:HD3	2:E:112:SER:HB3	1.91	0.52
1:D:129:PHE:HA	1:D:144:GLU:O	2.10	0.52
1:H:28:GLU:C	1:H:30:GLN:H	2.14	0.51
1:D:92:GLN:HB2	1:D:104:THR:CB	2.41	0.51
2:E:33:GLU:HB3	2:E:95:LEU:HD13	1.93	0.51
1:H:26:CYS:HB2	1:H:31:TYR:HA	1.93	0.51
2:G:22:CYS:HB3	2:G:78:LEU:HB3	1.93	0.51
2:I:22:CYS:HB3	2:I:78:LEU:HB3	1.92	0.51
2:E:22:CYS:HB3	2:E:78:LEU:HB3	1.92	0.51
1:D:157:ALA:HB3	2:E:33:GLU:OE1	2.11	0.50
1:A:105:CYS:SG	1:A:111:CYS:HA	2.52	0.50
1:F:35:SER:HA	1:F:36:GLN:C	2.31	0.50
1:F:81:LYS:O	1:F:82:TYR:HB3	2.12	0.50
1:H:129:PHE:HA	1:H:144:GLU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:HIS:HB3	2:G:47:ARG:HH21	1.76	0.49
1:A:121:LEU:HB3	2:B:97:PHE:HB3	1.93	0.49
1:F:131:VAL:HA	1:F:143:CYS:HB3	1.94	0.48
1:F:150:PHE:HB3	1:F:161:CYS:SG	2.53	0.48
1:H:128:GLY:CA	1:H:129:PHE:HB2	2.43	0.48
1:D:128:GLY:HA3	1:D:129:PHE:CB	2.44	0.48
2:I:30:ARG:O	2:I:52(A):PRO:HB2	2.13	0.48
1:H:26:CYS:HB3	1:H:30:GLN:OE1	2.13	0.47
1:F:126:SER:HA	1:F:128:GLY:H	1.79	0.47
1:F:89:LEU:HD22	1:F:103:CYS:HB3	1.97	0.47
2:B:12:VAL:O	2:B:111:VAL:HA	2.15	0.47
1:F:127:PRO:HA	1:F:152:SER:O	2.15	0.46
2:I:12:VAL:O	2:I:111:VAL:HA	2.15	0.46
1:F:136:THR:CA	1:F:138:VAL:H	2.29	0.46
1:H:165:THR:H	1:H:184:VAL:HG11	1.81	0.46
2:B:95:LEU:O	2:B:96:PRO:C	2.53	0.46
1:A:136:THR:CA	1:A:138:VAL:H	2.29	0.45
1:H:32:LEU:HD13	1:H:38:CYS:HB2	1.97	0.45
1:D:160:LYS:H	2:E:56:ARG:NH1	2.15	0.45
1:H:111:CYS:HB3	1:H:116:CYS:HA	1.98	0.45
1:H:146:CYS:SG	1:H:146:CYS:O	2.73	0.45
1:A:81:LYS:HB2	1:A:101:THR:HB	1.99	0.45
1:F:162:HIS:HE1	2:G:56:ARG:CD	2.30	0.45
1:F:126:SER:HA	1:F:128:GLY:N	2.32	0.45
1:D:131:VAL:HG12	1:D:133:GLN:H	1.82	0.45
1:A:83:CYS:HB3	1:A:89:LEU:HB3	1.98	0.44
2:G:96:PRO:O	2:G:97:PHE:CD2	2.70	0.44
1:H:110:HIS:CG	1:H:139:SER:HB3	2.52	0.44
1:D:24:THR:HG23	1:D:26:CYS:H	1.82	0.44
1:A:136:THR:HA	1:A:138:VAL:H	1.83	0.44
1:D:130:GLY:O	1:D:143:CYS:HA	2.17	0.44
1:H:119:CYS:HB2	2:I:99:PHE:HE1	1.83	0.44
1:A:136:THR:CA	1:A:138:VAL:N	2.79	0.44
1:A:110:HIS:HB2	1:A:139:SER:O	2.18	0.43
1:A:131:VAL:HG13	1:A:133:GLN:H	1.83	0.43
1:D:41:CYS:O	1:D:71:TRP:HA	2.19	0.43
1:D:68:LEU:HA	1:D:68:LEU:HD23	1.95	0.43
2:I:63:VAL:HA	2:I:66:ARG:HH21	1.84	0.43
1:A:177:ALA:HB1	1:A:181:LYS:O	2.18	0.43
1:A:28:GLU:O	1:A:29:LYS:HB2	2.19	0.43
1:D:32:LEU:HD22	1:D:38:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ASP:HB3	1:F:87:LEU:HB2	2.00	0.43
1:F:162:HIS:HE1	2:G:56:ARG:HD2	1.83	0.43
2:G:63:VAL:HA	2:G:66:ARG:HH21	1.84	0.43
1:H:95:GLY:H	1:H:101:THR:HB	1.84	0.43
1:F:24:THR:HG22	1:F:25:ALA:H	1.84	0.43
1:D:72:ASN:HB2	1:D:74:GLU:HG3	2.02	0.42
2:I:87:THR:HG23	2:I:110:THR:HA	2.00	0.42
1:A:66:GLU:HB3	1:A:77:CYS:CB	2.50	0.42
1:A:41:CYS:O	1:A:71:TRP:HA	2.19	0.42
2:E:63:VAL:HA	2:E:66:ARG:HH21	1.85	0.42
1:F:112:THR:HG22	1:F:120:VAL:HB	2.01	0.42
2:B:11:LEU:HA	2:B:110:THR:O	2.18	0.42
1:A:49:SER:HA	1:D:33:ILE:HG23	2.02	0.42
2:B:89:VAL:HG22	2:B:108:LEU:HD13	2.01	0.42
1:D:33:ILE:HG12	1:D:36:GLN:O	2.20	0.42
1:F:41:CYS:O	1:F:71:TRP:HA	2.19	0.42
1:H:81:LYS:HB2	1:H:101:THR:HG23	2.00	0.42
1:F:83:CYS:HB3	1:F:89:LEU:HB3	2.02	0.42
1:H:68:LEU:HA	1:H:68:LEU:HD23	1.96	0.42
1:H:41:CYS:O	1:H:71:TRP:HA	2.19	0.42
1:A:176:GLN:HA	1:A:184:VAL:HG12	2.01	0.41
2:E:95:LEU:HD23	2:E:96:PRO:HB3	2.02	0.41
1:H:84:ASP:HA	1:H:85:PRO:HD3	1.90	0.41
1:H:110:HIS:CD2	1:H:139:SER:HB3	2.55	0.41
2:E:87:THR:OG1	2:E:111:VAL:HG22	2.20	0.41
1:F:124:SER:HB3	2:G:95:LEU:HD11	2.02	0.41
1:A:63:GLY:C	1:A:65:SER:H	2.23	0.41
1:H:51:CYS:H	1:H:57:THR:HG23	1.85	0.41
1:D:122:HIS:NE2	2:E:47:ARG:HG2	2.36	0.41
1:H:138:VAL:C	1:H:140:ASP:H	2.25	0.41
2:G:87:THR:HG23	2:G:110:THR:HA	2.02	0.40
2:I:40:ALA:HB3	2:I:43:LYS:HB2	2.02	0.40
1:A:72:ASN:HB2	1:A:74:GLU:HG3	2.04	0.40
1:F:172:LEU:O	1:F:173:VAL:HG23	2.21	0.40
1:H:128:GLY:HA3	1:H:129:PHE:CB	2.52	0.40

There are no symmetry-related clashes.

## 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	166/183 (91%)	120 (72%)	21 (13%)	25 (15%)	0	1
1	D	163/183 (89%)	111 (68%)	31 (19%)	21 (13%)	0	2
1	F	163/183 (89%)	115 (71%)	26 (16%)	22 (14%)	0	2
1	H	165/183 (90%)	120 (73%)	23 (14%)	22 (13%)	0	2
2	B	115/121 (95%)	102 (89%)	9 (8%)	4 (4%)	4	26
2	E	116/121 (96%)	105 (90%)	9 (8%)	2 (2%)	11	42
2	G	115/121 (95%)	103 (90%)	7 (6%)	5 (4%)	3	21
2	I	115/121 (95%)	105 (91%)	7 (6%)	3 (3%)	6	33
All	All	1118/1216 (92%)	881 (79%)	133 (12%)	104 (9%)	1	5

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	154	VAL
1	A	168	GLU
1	A	179	THR
1	A	185	VAL
1	A	186	CYS
2	B	44	GLY
2	B	45	LEU
1	D	116	CYS
1	D	133	GLN
1	D	177	ALA
2	E	44	GLY
2	E	45	LEU
1	F	35	SER
1	F	36	GLN
1	F	82	TYR
1	F	129	PHE

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Mol	Chain	Res	Type
1	F	139	SER
1	F	142	ILE
1	F	172	LEU
1	F	173	VAL
1	F	185	VAL
2	G	44	GLY
2	G	45	LEU
2	G	97	PHE
1	H	122	HIS
1	H	129	PHE
1	H	134	ILE
1	H	142	ILE
1	H	154	VAL
2	I	44	GLY
2	I	45	LEU
1	A	106	GLU
1	A	136	THR
1	A	142	ILE
1	A	169	THR
1	A	183	ASP
1	A	189	GLN
1	D	106	GLU
1	D	107	GLU
1	D	129	PHE
1	D	146	CYS
1	D	157	ALA
1	D	173	VAL
1	F	107	GLU
1	F	116	CYS
1	F	128	GLY
1	F	154	VAL
1	F	168	GLU
1	F	184	VAL
2	G	112	SER
1	H	31	TYR
1	H	34	ASN
1	H	116	CYS
1	H	177	ALA
2	I	102	ASP
1	A	25	ALA
1	A	107	GLU
1	A	125	CYS

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Mol	Chain	Res	Type
1	A	127	PRO
2	B	102	ASP
1	D	31	TYR
1	D	35	SER
1	D	179	THR
1	F	25	ALA
1	F	133	GLN
1	F	136	THR
1	H	32	LEU
1	H	107	GLU
1	H	115	ALA
1	H	136	THR
1	H	151	PHE
1	A	26	CYS
1	A	29	LYS
1	D	115	ALA
1	D	137	GLY
1	D	139	SER
1	F	32	LEU
1	F	115	ALA
1	H	139	SER
1	H	146	CYS
1	H	179	THR
1	A	35	SER
1	A	133	GLN
1	D	142	ILE
1	D	172	LEU
1	H	170	LYS
1	H	171	ASP
1	H	184	VAL
1	A	32	LEU
2	B	95	LEU
1	D	83	CYS
1	D	128	GLY
2	G	102	ASP
1	H	29	LYS
1	H	173	VAL
1	A	188	PRO
1	F	126	SER
1	A	138	VAL
1	A	184	VAL
1	D	178	GLY

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Mol	Chain	Res	Type
1	F	33	ILE
1	A	178	GLY
1	D	145	PRO

### 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	132/162 (82%)	112 (85%)	20 (15%)	3	16
1	D	109/162 (67%)	95 (87%)	14 (13%)	5	22
1	F	122/162 (75%)	105 (86%)	17 (14%)	4	20
1	H	117/162 (72%)	97 (83%)	20 (17%)	2	11
2	B	91/98 (93%)	79 (87%)	12 (13%)	5	21
2	E	90/98 (92%)	79 (88%)	11 (12%)	6	25
2	G	91/98 (93%)	83 (91%)	8 (9%)	12	40
2	I	92/98 (94%)	83 (90%)	9 (10%)	9	34
All	All	844/1040 (81%)	733 (87%)	111 (13%)	5	21

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	CYS
1	A	37	CYS
1	A	39	SER
1	A	51	CYS
1	A	57	THR
1	A	58	GLU
1	A	68	LEU
1	A	98	GLU
1	A	110	HIS
1	A	111	CYS
1	A	116	CYS
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	127	PRO
1	A	141	THR
1	A	153	ASP
1	A	154	VAL
1	A	155	SER
1	A	168	GLU
1	A	171	ASP
1	A	175	GLN
2	B	4	LEU
2	B	6	GLU
2	B	19	ARG
2	B	28	THR
2	B	33	GLU
2	B	47	ARG
2	B	53	GLN
2	B	64	MET
2	B	70	SER
2	B	86	ASP
2	B	101	ASP
2	B	110	THR
1	D	26	CYS
1	D	30	GLN
1	D	33	ILE
1	D	39	SER
1	D	49	SER
1	D	51	CYS
1	D	57	THR
1	D	97	SER
1	D	98	GLU
1	D	111	CYS
1	D	114	GLU
1	D	133	GLN
1	D	141	THR
1	D	165	THR
2	E	4	LEU
2	E	6	GLU
2	E	28	THR
2	E	64	MET
2	E	70	SER
2	E	82	MET
2	E	86	ASP
2	E	95	LEU

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Mol	Chain	Res	Type
2	E	101	ASP
2	E	102	ASP
2	E	110	THR
1	F	26	CYS
1	F	35	SER
1	F	36	GLN
1	F	37	CYS
1	F	39	SER
1	F	51	CYS
1	F	57	THR
1	F	58	GLU
1	F	68	LEU
1	F	99	THR
1	F	110	HIS
1	F	111	CYS
1	F	113	SER
1	F	132	LYS
1	F	139	SER
1	F	153	ASP
1	F	155	SER
2	G	4	LEU
2	G	6	GLU
2	G	47	ARG
2	G	64	MET
2	G	70	SER
2	G	86	ASP
2	G	101	ASP
2	G	102	ASP
1	H	27	ARG
1	H	30	GLN
1	H	33	ILE
1	H	39	SER
1	H	49	SER
1	H	51	CYS
1	H	57	THR
1	H	65	SER
1	H	87	LEU
1	H	97	SER
1	H	98	GLU
1	H	101	THR
1	H	110	HIS
1	H	113	SER

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Mol	Chain	Res	Type
1	H	124	SER
1	H	139	SER
1	H	141	THR
1	H	142	ILE
1	H	143	CYS
1	H	146	CYS
2	I	6	GLU
2	I	7	SER
2	I	28	THR
2	I	31	ASP
2	I	64	MET
2	I	70	SER
2	I	82	MET
2	I	95	LEU
2	I	101	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	HIS
1	H	122	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	301	-	4,4,4	0.27	0	6,6,6	0.38	0
3	SO4	A	302	-	4,4,4	0.31	0	6,6,6	0.31	0
3	SO4	B	201	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	G	201	-	4,4,4	0.16	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	301	-	-	0/0/0/0	0/0/0/0
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
3	SO4	B	201	-	-	0/0/0/0	0/0/0/0
3	SO4	G	201	-	-	0/0/0/0	0/0/0/0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 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	168/183 (91%)	-0.09	2 (1%) 79 77	27, 59, 94, 132	0
1	D	165/183 (90%)	0.17	9 (5%) 26 24	45, 93, 153, 167	0
1	F	165/183 (90%)	0.21	8 (4%) 31 29	39, 88, 176, 183	0
1	H	167/183 (91%)	0.08	7 (4%) 37 34	31, 88, 174, 182	0
2	B	117/121 (96%)	-0.28	0 100 100	20, 60, 86, 113	0
2	E	118/121 (97%)	-0.04	2 (1%) 70 67	60, 86, 123, 149	0
2	G	117/121 (96%)	-0.22	0 100 100	38, 68, 109, 136	0
2	I	117/121 (96%)	-0.27	2 (1%) 70 67	32, 63, 110, 123	0
All	All	1134/1216 (93%)	-0.03	30 (2%) 56 53	20, 77, 149, 183	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	189	GLN	4.6
1	H	176	GLN	4.2
1	F	166	SER	3.8
1	D	184	VAL	3.7
1	H	177	ALA	3.7
2	E	24	ALA	3.3
1	D	186	CYS	3.3
1	D	166	SER	3.3
1	F	176	GLN	3.3
1	D	177	ALA	3.2
1	F	167	CYS	3.2
1	D	171	ASP	3.1
1	H	167	CYS	3.0
1	H	166	SER	3.0
1	F	188	PRO	3.0
1	H	188	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	186	CYS	2.9
1	D	176	GLN	2.7
1	D	185	VAL	2.6
2	E	23	ALA	2.6
1	F	165	THR	2.5
1	A	24	THR	2.4
2	I	-1	THR	2.4
1	D	82	TYR	2.2
1	D	167	CYS	2.2
1	F	185	VAL	2.2
1	A	25	ALA	2.2
1	F	133	GLN	2.1
1	H	173	VAL	2.1
2	I	24	ALA	2.1

## 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 carbohydrates 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	302	5/5	0.93	0.18	0.70	92,93,96,101	0
3	SO4	A	301	5/5	0.95	0.18	0.27	50,51,55,56	0
3	SO4	B	201	5/5	0.96	0.14	-2.88	94,98,99,105	0
3	SO4	G	201	5/5	0.94	0.12	-4.38	115,117,120,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.