



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 AM GMT

PDB ID : 2V3M  
Title : STRUCTURE OF THE GAR1 DOMAIN OF NAF1  
Authors : Leulliot, N.; Godin, K.S.; Hoareau-Aveilla, C.; Quevillon-Cheruel, S.; Varani, G.; Henry, Y.; Van Tilbeurgh, H.  
Deposited on : 2007-06-19  
Resolution : 2.74 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 (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

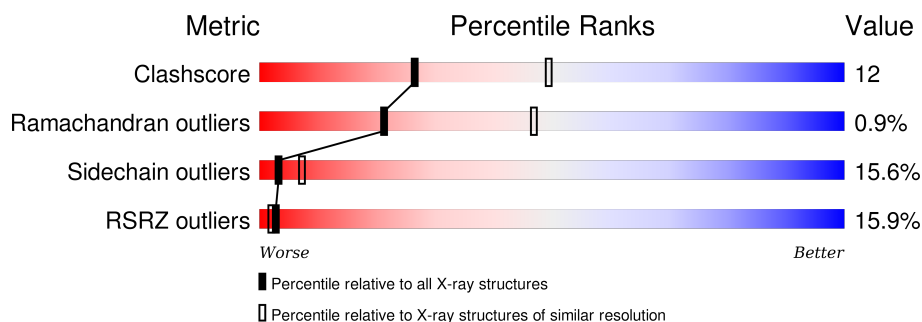
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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))
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	131	
1	B	131	
1	C	131	
1	D	131	
1	E	131	
1	F	131	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4576 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 NAF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	Se	0	0	0
			754	492	121	139	1	1			
1	B	86	Total	C	N	O	S	Se	0	0	0
			694	455	109	128	1	1			
1	C	101	Total	C	N	O	S	Se	0	0	0
			806	522	129	152	1	2			
1	D	94	Total	C	N	O	S	Se	0	0	0
			752	491	118	141	1	1			
1	E	101	Total	C	N	O	S	Se	0	0	0
			806	522	129	152	1	2			
1	F	91	Total	C	N	O	S	Se	0	0	0
			729	476	115	136	1	1			

There are 42 discrepancies between the modelled and reference sequences:

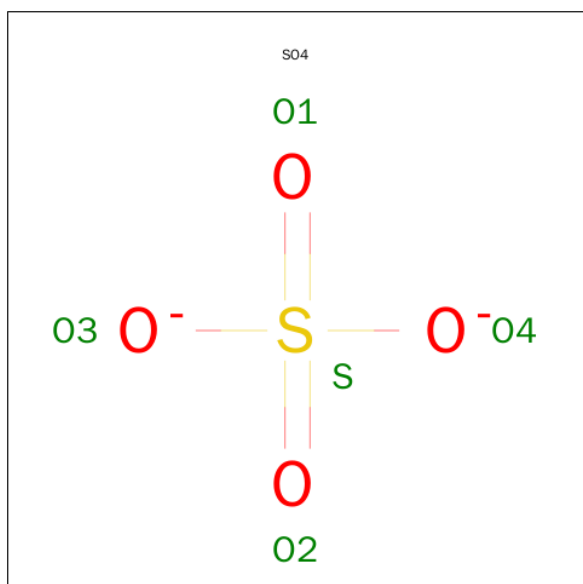
Chain	Residue	Modelled	Actual	Comment	Reference
A	108	MSE	-	EXPRESSION TAG	UNP P53919
A	233	HIS	-	EXPRESSION TAG	UNP P53919
A	234	HIS	-	EXPRESSION TAG	UNP P53919
A	235	HIS	-	EXPRESSION TAG	UNP P53919
A	236	HIS	-	EXPRESSION TAG	UNP P53919
A	237	HIS	-	EXPRESSION TAG	UNP P53919
A	238	HIS	-	EXPRESSION TAG	UNP P53919
B	108	MSE	-	EXPRESSION TAG	UNP P53919
B	233	HIS	-	EXPRESSION TAG	UNP P53919
B	234	HIS	-	EXPRESSION TAG	UNP P53919
B	235	HIS	-	EXPRESSION TAG	UNP P53919
B	236	HIS	-	EXPRESSION TAG	UNP P53919
B	237	HIS	-	EXPRESSION TAG	UNP P53919
B	238	HIS	-	EXPRESSION TAG	UNP P53919
C	108	MSE	-	EXPRESSION TAG	UNP P53919
C	233	HIS	-	EXPRESSION TAG	UNP P53919
C	234	HIS	-	EXPRESSION TAG	UNP P53919

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Chain	Residue	Modelled	Actual	Comment	Reference
C	235	HIS	-	EXPRESSION TAG	UNP P53919
C	236	HIS	-	EXPRESSION TAG	UNP P53919
C	237	HIS	-	EXPRESSION TAG	UNP P53919
C	238	HIS	-	EXPRESSION TAG	UNP P53919
D	108	MSE	-	EXPRESSION TAG	UNP P53919
D	233	HIS	-	EXPRESSION TAG	UNP P53919
D	234	HIS	-	EXPRESSION TAG	UNP P53919
D	235	HIS	-	EXPRESSION TAG	UNP P53919
D	236	HIS	-	EXPRESSION TAG	UNP P53919
D	237	HIS	-	EXPRESSION TAG	UNP P53919
D	238	HIS	-	EXPRESSION TAG	UNP P53919
E	108	MSE	-	EXPRESSION TAG	UNP P53919
E	233	HIS	-	EXPRESSION TAG	UNP P53919
E	234	HIS	-	EXPRESSION TAG	UNP P53919
E	235	HIS	-	EXPRESSION TAG	UNP P53919
E	236	HIS	-	EXPRESSION TAG	UNP P53919
E	237	HIS	-	EXPRESSION TAG	UNP P53919
E	238	HIS	-	EXPRESSION TAG	UNP P53919
F	108	MSE	-	EXPRESSION TAG	UNP P53919
F	233	HIS	-	EXPRESSION TAG	UNP P53919
F	234	HIS	-	EXPRESSION TAG	UNP P53919
F	235	HIS	-	EXPRESSION TAG	UNP P53919
F	236	HIS	-	EXPRESSION TAG	UNP P53919
F	237	HIS	-	EXPRESSION TAG	UNP P53919
F	238	HIS	-	EXPRESSION TAG	UNP P53919

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

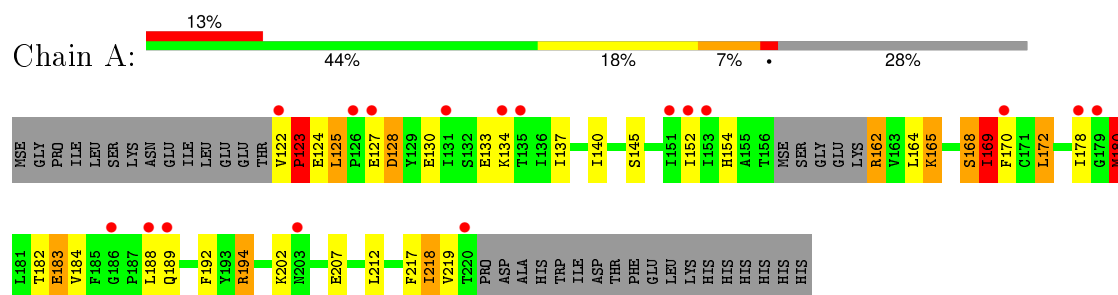


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

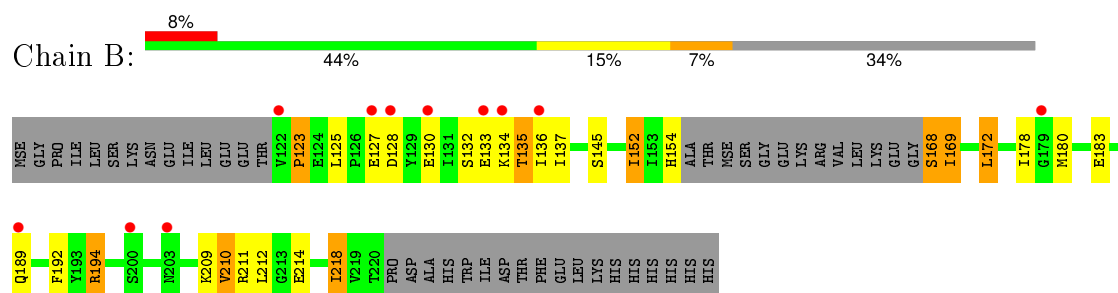
### 3 Residue-property plots [i](#)

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

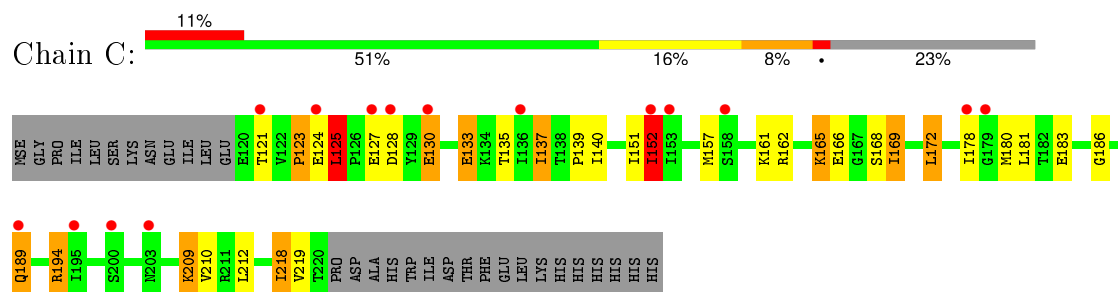
#### • Molecule 1: NAF1



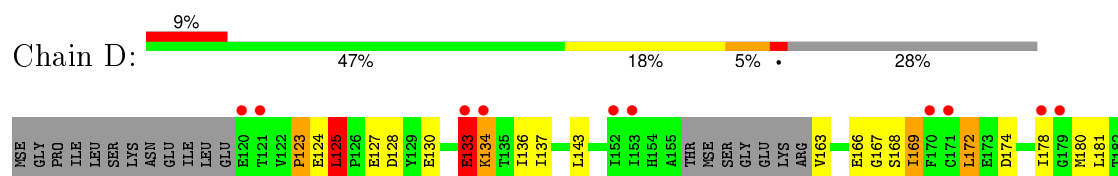
#### • Molecule 1: NAF1



#### • Molecule 1: NAF1

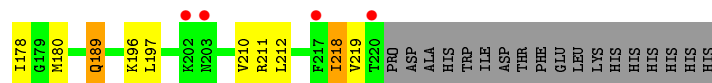
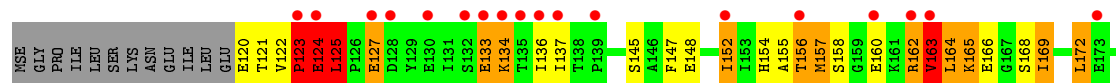


#### • Molecule 1: NAF1

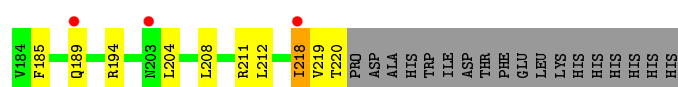
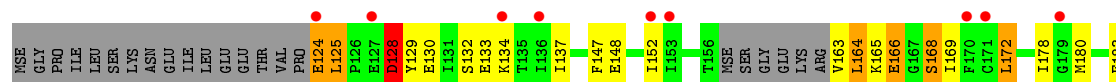
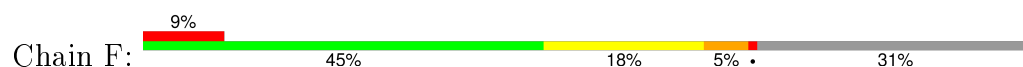




• Molecule 1: NAF1



• Molecule 1: NAF1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.53Å 103.53Å 109.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.57 – 2.74 19.61 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.57-2.74) 99.3 (19.61-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.257 , 0.287 0.283 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 13.8	EDS
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18001 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.24% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 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	1.49	7/766 (0.9%)	1.34	8/1032 (0.8%)
1	B	1.31	7/706 (1.0%)	1.26	11/952 (1.2%)
1	C	1.43	9/818 (1.1%)	1.31	10/1100 (0.9%)
1	D	1.46	7/764 (0.9%)	1.25	7/1030 (0.7%)
1	E	1.26	7/818 (0.9%)	1.13	8/1100 (0.7%)
1	F	1.63	14/740 (1.9%)	1.40	10/996 (1.0%)
All	All	1.43	51/4612 (1.1%)	1.28	54/6210 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	124	GLU	CB-CG	-12.40	1.28	1.52
1	C	124	GLU	CB-CG	-11.18	1.30	1.52
1	D	124	GLU	CB-CG	-10.62	1.31	1.52
1	E	133	GLU	CD-OE1	-10.21	1.14	1.25
1	F	134	LYS	CB-CG	-9.72	1.26	1.52
1	B	128	ASP	CB-CG	-9.61	1.31	1.51
1	F	128	ASP	CB-CG	-9.45	1.31	1.51
1	D	130	GLU	CB-CG	-9.36	1.34	1.52
1	F	124	GLU	CB-CG	-9.04	1.34	1.52
1	C	124	GLU	CA-CB	-8.04	1.36	1.53
1	C	127	GLU	CB-CG	-7.84	1.37	1.52
1	F	166	GLU	CD-OE1	7.52	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	GLU	CD-OE1	-7.50	1.17	1.25
1	D	133	GLU	CD-OE1	-7.40	1.17	1.25
1	A	130	GLU	CB-CG	-7.31	1.38	1.52
1	F	133	GLU	CD-OE1	-7.20	1.17	1.25
1	A	124	GLU	CB-CG	-7.06	1.38	1.52
1	F	134	LYS	CG-CD	-6.76	1.29	1.52
1	B	127	GLU	CB-CG	-6.70	1.39	1.52
1	E	124	GLU	CG-CD	-6.63	1.42	1.51
1	F	124	GLU	CA-CB	-6.57	1.39	1.53
1	D	134	LYS	CB-CG	-6.42	1.35	1.52
1	E	127	GLU	CB-CG	-6.36	1.40	1.52
1	A	127	GLU	CB-CG	-6.28	1.40	1.52
1	C	130	GLU	CB-CG	-6.23	1.40	1.52
1	F	129	TYR	CE1-CZ	6.22	1.46	1.38
1	C	135	THR	CB-CG2	-6.22	1.31	1.52
1	F	133	GLU	CG-CD	-6.20	1.42	1.51
1	A	134	LYS	CB-CG	-6.19	1.35	1.52
1	A	133	GLU	CD-OE1	-6.19	1.18	1.25
1	F	125	LEU	CG-CD2	-6.14	1.29	1.51
1	A	207	GLU	CG-CD	6.10	1.61	1.51
1	A	125	LEU	CG-CD1	-6.00	1.29	1.51
1	B	133	GLU	CD-OE1	-5.94	1.19	1.25
1	C	125	LEU	CG-CD1	-5.76	1.30	1.51
1	D	124	GLU	CG-CD	-5.75	1.43	1.51
1	B	134	LYS	CE-NZ	-5.67	1.34	1.49
1	B	134	LYS	CD-CE	-5.65	1.37	1.51
1	F	133	GLU	CD-OE2	-5.62	1.19	1.25
1	E	125	LEU	CG-CD1	-5.58	1.31	1.51
1	F	125	LEU	CG-CD1	-5.52	1.31	1.51
1	C	125	LEU	CG-CD2	-5.50	1.31	1.51
1	E	163	VAL	CA-CB	5.48	1.66	1.54
1	F	185	PHE	CD2-CE2	5.31	1.49	1.39
1	C	133	GLU	CD-OE2	-5.27	1.19	1.25
1	E	124	GLU	CA-CB	-5.20	1.42	1.53
1	B	125	LEU	CG-CD1	-5.16	1.32	1.51
1	D	134	LYS	CD-CE	-5.09	1.38	1.51
1	F	183	GLU	CD-OE2	5.07	1.31	1.25
1	B	128	ASP	CG-OD1	-5.06	1.13	1.25
1	D	217	PHE	CE1-CZ	5.01	1.46	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	LYS	CD-CE-NZ	12.31	140.01	111.70
1	B	128	ASP	CB-CG-OD1	-11.26	108.16	118.30
1	F	134	LYS	CD-CE-NZ	-11.25	85.82	111.70
1	A	180	MSE	CB-CG-SE	-9.38	84.55	112.70
1	F	128	ASP	CB-CA-C	-9.33	91.73	110.40
1	B	194	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	128	ASP	CB-CG-OD2	7.64	125.17	118.30
1	C	124	GLU	N-CA-C	7.54	131.35	111.00
1	C	128	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	125	LEU	CA-CB-CG	7.41	132.34	115.30
1	F	194	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	128	ASP	N-CA-CB	-7.25	97.55	110.60
1	C	194	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	F	124	GLU	N-CA-CB	-7.19	97.66	110.60
1	D	128	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	194	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	164	LEU	CA-CB-CG	6.74	130.79	115.30
1	E	125	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	C	152	ILE	CA-CB-CG1	-6.67	98.33	111.00
1	E	134	LYS	CD-CE-NZ	-6.54	96.67	111.70
1	A	183	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	B	125	LEU	CB-CG-CD2	6.43	121.94	111.00
1	D	125	LEU	CA-CB-CG	6.41	130.04	115.30
1	F	164	LEU	CA-CB-CG	6.38	129.97	115.30
1	E	124	GLU	N-CA-C	6.33	128.09	111.00
1	A	128	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	A	194	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	C	152	ILE	CG1-CB-CG2	6.12	124.87	111.40
1	B	125	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	133	GLU	CA-CB-CG	-5.90	100.41	113.40
1	F	128	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	D	124	GLU	CG-CD-OE1	-5.67	106.97	118.30
1	F	124	GLU	N-CA-C	5.64	126.24	111.00
1	A	128	ASP	CB-CG-OD2	5.59	123.33	118.30
1	E	136	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	E	123	PRO	C-N-CA	-5.56	107.80	121.70
1	E	164	LEU	N-CA-C	5.56	126.01	111.00
1	D	123	PRO	C-N-CA	5.50	135.45	121.70
1	C	124	GLU	N-CA-CB	-5.48	100.73	110.60
1	C	181	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	D	181	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	B	123	PRO	C-N-CA	5.39	135.17	121.70
1	A	169	ILE	CB-CA-C	-5.35	100.90	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	F	166	GLU	CG-CD-OE1	5.26	128.82	118.30
1	F	166	GLU	CG-CD-OE2	-5.24	107.82	118.30
1	D	124	GLU	CB-CA-C	-5.22	99.95	110.40
1	E	124	GLU	N-CA-CB	-5.17	101.29	110.60
1	E	152	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	B	133	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	133	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	C	135	THR	OG1-CB-CG2	-5.09	98.29	110.00
1	F	211	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	134	LYS	CG-CD-CE	-5.00	96.90	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	163	VAL	Peptide

## 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	754	0	785	22	0
1	B	694	0	718	20	0
1	C	806	0	835	18	0
1	D	752	0	778	30	0
1	E	806	0	835	31	1
1	F	729	0	756	15	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
All	All	4576	0	4707	113	1

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 12.

All (113) 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:E:165:LYS:CD	1:E:165:LYS:H	1.63	1.09
1:E:165:LYS:N	1:E:165:LYS:HD2	1.70	1.04
1:E:165:LYS:HD2	1:E:165:LYS:H	0.86	0.99
1:B:209:LYS:HE2	1:D:133:GLU:HG3	1.46	0.96
1:C:165:LYS:HE2	1:C:165:LYS:H	1.31	0.92
1:E:123:PRO:O	1:E:124:GLU:HB2	1.81	0.80
1:A:154:HIS:ND1	1:F:148:GLU:OE2	2.14	0.79
1:A:123:PRO:HB2	1:A:180:MSE:HE2	1.65	0.78
1:E:168:SER:HB3	1:E:218:ILE:HD11	1.65	0.77
1:C:165:LYS:HE2	1:C:165:LYS:N	2.00	0.76
1:D:169:ILE:HD13	1:D:169:ILE:N	2.00	0.75
1:E:165:LYS:O	1:E:168:SER:OG	2.06	0.73
1:D:168:SER:HB3	1:D:218:ILE:HD11	1.70	0.73
1:F:168:SER:HB3	1:F:218:ILE:HD11	1.71	0.73
1:B:209:LYS:HG2	1:D:133:GLU:CG	2.20	0.72
1:B:123:PRO:HB2	1:B:180:MSE:SE	2.40	0.71
1:B:183:GLU:OE1	1:B:194:ARG:NH1	2.21	0.71
1:A:188:LEU:HD13	1:D:166:GLU:HA	1.71	0.71
1:A:168:SER:HB3	1:A:218:ILE:HD11	1.75	0.68
1:C:121:THR:O	1:C:123:PRO:HD3	1.93	0.68
1:B:209:LYS:HG2	1:D:133:GLU:HG2	1.77	0.67
1:C:161:LYS:HD3	1:C:189:GLN:O	1.95	0.67
1:E:154:HIS:ND1	1:E:156:THR:OG1	2.28	0.66
1:D:167:GLY:HA2	1:D:180:MSE:HG2	1.77	0.65
1:E:169:ILE:HD13	1:E:169:ILE:N	2.14	0.63
1:F:125:LEU:HD21	1:F:180:MSE:HE3	1.80	0.63
1:B:168:SER:HB3	1:B:218:ILE:HD11	1.80	0.62
1:F:218:ILE:HD13	1:F:219:VAL:N	2.14	0.62
1:D:183:GLU:OE1	1:D:194:ARG:NH1	2.33	0.61
1:A:140:ILE:HD12	1:A:162:ARG:HB3	1.83	0.59
1:D:136:ILE:HD12	1:E:210:VAL:O	2.03	0.58
1:A:188:LEU:HB3	1:D:166:GLU:HB3	1.83	0.58
1:C:169:ILE:N	1:C:169:ILE:HD13	2.18	0.58
1:A:128:ASP:N	1:A:128:ASP:OD1	2.30	0.58
1:B:210:VAL:HG13	1:D:174:ASP:HB2	1.86	0.58
1:A:169:ILE:HD13	1:A:169:ILE:N	2.20	0.57
1:A:165:LYS:O	1:A:168:SER:OG	2.22	0.57
1:E:169:ILE:CD1	1:E:169:ILE:N	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:HIS:ND1	1:E:148:GLU:OE2	2.37	0.57
1:A:183:GLU:OE1	1:A:194:ARG:NH1	2.36	0.56
1:C:183:GLU:OE1	1:C:194:ARG:NH1	2.38	0.55
1:D:172:LEU:HD13	1:D:178:ILE:HD11	1.87	0.55
1:E:125:LEU:CD2	1:E:180:MSE:HE3	2.38	0.54
1:E:155:ALA:O	1:E:157:MSE:N	2.40	0.54
1:A:218:ILE:HD13	1:A:219:VAL:N	2.23	0.54
1:E:154:HIS:CE1	1:E:156:THR:OG1	2.60	0.54
1:F:165:LYS:O	1:F:168:SER:OG	2.26	0.53
1:B:172:LEU:HD13	1:B:178:ILE:HD11	1.91	0.53
1:A:172:LEU:HD13	1:A:178:ILE:HD11	1.90	0.53
1:E:147:PHE:HA	2:E:1221:SO4:O2	2.09	0.53
1:B:192:PHE:CE2	1:E:147:PHE:HE1	2.26	0.53
1:E:120:GLU:C	1:E:122:VAL:H	2.12	0.53
1:A:145:SER:HB3	1:A:152:ILE:HB	1.92	0.52
1:C:168:SER:HB3	1:C:218:ILE:HD11	1.91	0.52
1:C:139:PRO:HB2	1:C:157:MSE:HE1	1.91	0.52
1:B:209:LYS:CE	1:D:133:GLU:HG3	2.32	0.52
1:E:172:LEU:HD13	1:E:178:ILE:HD11	1.92	0.52
1:B:209:LYS:HE2	1:D:133:GLU:CG	2.29	0.52
1:E:154:HIS:CG	1:E:156:THR:OG1	2.62	0.52
1:B:169:ILE:HD13	1:B:169:ILE:N	2.25	0.51
1:E:218:ILE:HD13	1:E:219:VAL:N	2.23	0.51
1:D:167:GLY:HA2	1:D:180:MSE:CG	2.40	0.51
1:F:218:ILE:HD13	1:F:218:ILE:C	2.31	0.51
1:E:122:VAL:HG23	1:E:196:LYS:O	2.11	0.50
1:C:186:GLY:N	1:D:183:GLU:OE2	2.28	0.50
1:A:154:HIS:HD1	1:F:148:GLU:CD	2.13	0.50
1:E:162:ARG:O	1:E:165:LYS:HE3	2.11	0.50
1:D:169:ILE:CD1	1:D:169:ILE:N	2.69	0.49
1:C:218:ILE:HD13	1:C:219:VAL:N	2.28	0.49
1:E:155:ALA:C	1:E:157:MSE:N	2.66	0.49
1:D:123:PRO:O	1:D:180:MSE:SE	2.82	0.48
1:F:172:LEU:HD13	1:F:178:ILE:HD11	1.96	0.48
1:B:145:SER:OG	1:E:145:SER:OG	2.30	0.48
1:A:188:LEU:HB3	1:D:166:GLU:CB	2.44	0.47
1:E:178:ILE:O	1:E:197:LEU:HD21	2.15	0.47
1:A:125:LEU:CD2	1:A:180:MSE:SE	3.13	0.47
1:D:218:ILE:HD13	1:D:219:VAL:N	2.30	0.47
1:C:125:LEU:HD11	1:C:180:MSE:HE3	1.98	0.46
1:C:218:ILE:HD12	1:C:219:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE2	1:F:147:PHE:HE1	2.34	0.46
1:D:125:LEU:HD13	1:D:180:MSE:HE3	1.98	0.46
1:F:128:ASP:OD1	1:F:128:ASP:N	2.48	0.46
1:C:151:ILE:C	1:C:152:ILE:HG12	2.35	0.46
1:B:211:ARG:HD2	1:B:214:GLU:OE2	2.16	0.45
1:C:162:ARG:HG2	1:F:163:VAL:HG11	1.98	0.45
1:B:169:ILE:CD1	1:B:169:ILE:N	2.79	0.45
1:C:165:LYS:NZ	1:F:163:VAL:HG13	2.31	0.45
1:F:219:VAL:HG12	1:F:220:THR:N	2.31	0.44
1:C:137:ILE:HD12	1:C:137:ILE:HA	1.62	0.44
1:C:140:ILE:HA	1:C:140:ILE:HD12	1.84	0.44
1:D:219:VAL:HG12	1:D:220:THR:N	2.32	0.44
1:D:219:VAL:CG1	1:D:220:THR:N	2.81	0.43
1:D:218:ILE:HD12	1:D:219:VAL:O	2.18	0.43
1:B:145:SER:HB3	1:B:152:ILE:HB	2.00	0.43
1:A:184:VAL:HG21	1:D:163:VAL:HG13	2.00	0.43
1:F:204:LEU:O	1:F:208:LEU:HG	2.19	0.43
1:E:210:VAL:CG1	1:E:210:VAL:O	2.66	0.43
1:B:132:SER:HB3	1:B:135:THR:CG2	2.49	0.43
1:E:164:LEU:HD23	1:E:165:LYS:CD	2.48	0.43
1:B:194:ARG:NH2	2:B:1221:SO4:O4	2.52	0.43
1:A:182:THR:O	1:D:188:LEU:HD12	2.19	0.43
1:E:123:PRO:O	1:E:124:GLU:CB	2.50	0.42
1:F:219:VAL:CG1	1:F:220:THR:N	2.82	0.42
1:A:170:PHE:HA	1:A:217:PHE:O	2.20	0.42
1:D:143:LEU:HG	1:D:212:LEU:HD12	2.01	0.42
1:B:192:PHE:HE2	1:E:147:PHE:HE1	1.68	0.41
1:A:169:ILE:HD12	1:A:180:MSE:SE	2.70	0.41
1:D:168:SER:C	1:D:169:ILE:HD13	2.41	0.41
1:D:211:ARG:HD2	1:D:214:GLU:OE2	2.20	0.41
1:E:160:GLU:CG	1:E:160:GLU:O	2.69	0.41
1:A:182:THR:O	1:D:188:LEU:CD1	2.69	0.40
1:C:172:LEU:HD13	1:C:178:ILE:HD11	2.02	0.40
1:E:189:GLN:H	1:E:189:GLN:CD	2.23	0.40

All (1) 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)
1:E:163:VAL:O	1:E:163:VAL:O[4_465]	1.43	0.77

## 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	90/131 (69%)	85 (94%)	4 (4%)	1 (1%)	17	40
1	B	82/131 (63%)	78 (95%)	4 (5%)	0	100	100
1	C	99/131 (76%)	94 (95%)	5 (5%)	0	100	100
1	D	90/131 (69%)	86 (96%)	4 (4%)	0	100	100
1	E	99/131 (76%)	90 (91%)	5 (5%)	4 (4%)	4	7
1	F	87/131 (66%)	80 (92%)	7 (8%)	0	100	100
All	All	547/786 (70%)	513 (94%)	29 (5%)	5 (1%)	21	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	156	THR
1	E	158	SER
1	A	123	PRO
1	E	124	GLU
1	E	123	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	86/117 (74%)	73 (85%)	13 (15%)	3	8
1	B	80/117 (68%)	68 (85%)	12 (15%)	3	8
1	C	92/117 (79%)	77 (84%)	15 (16%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	86/117 (74%)	76 (88%)	10 (12%)	7	15
1	E	92/117 (79%)	75 (82%)	17 (18%)	2	4
1	F	83/117 (71%)	69 (83%)	14 (17%)	2	5
All	All	519/702 (74%)	438 (84%)	81 (16%)	3	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	123	PRO
1	A	137	ILE
1	A	162	ARG
1	A	165	LYS
1	A	168	SER
1	A	169	ILE
1	A	172	LEU
1	A	180	MSE
1	A	189	GLN
1	A	202	LYS
1	A	212	LEU
1	A	218	ILE
1	B	130	GLU
1	B	135	THR
1	B	136	ILE
1	B	137	ILE
1	B	152	ILE
1	B	168	SER
1	B	169	ILE
1	B	172	LEU
1	B	189	GLN
1	B	210	VAL
1	B	212	LEU
1	B	218	ILE
1	C	123	PRO
1	C	125	LEU
1	C	130	GLU
1	C	133	GLU
1	C	137	ILE
1	C	152	ILE
1	C	165	LYS
1	C	166	GLU

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Mol	Chain	Res	Type
1	C	169	ILE
1	C	172	LEU
1	C	189	GLN
1	C	209	LYS
1	C	210	VAL
1	C	212	LEU
1	C	218	ILE
1	D	125	LEU
1	D	127	GLU
1	D	133	GLU
1	D	134	LYS
1	D	137	ILE
1	D	169	ILE
1	D	172	LEU
1	D	189	GLN
1	D	212	LEU
1	D	218	ILE
1	E	121	THR
1	E	125	LEU
1	E	127	GLU
1	E	133	GLU
1	E	134	LYS
1	E	137	ILE
1	E	152	ILE
1	E	157	MSE
1	E	162	ARG
1	E	165	LYS
1	E	166	GLU
1	E	169	ILE
1	E	172	LEU
1	E	189	GLN
1	E	211	ARG
1	E	212	LEU
1	E	218	ILE
1	F	124	GLU
1	F	128	ASP
1	F	130	GLU
1	F	132	SER
1	F	137	ILE
1	F	152	ILE
1	F	164	LEU
1	F	166	GLU

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Mol	Chain	Res	Type
1	F	168	SER
1	F	169	ILE
1	F	172	LEU
1	F	189	GLN
1	F	212	LEU
1	F	218	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	203	ASN
1	C	203	ASN
1	D	203	ASN
1	E	203	ASN
1	F	203	ASN

### 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](#)

7 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	1221	-	4,4,4	0.24	0	6,6,6	0.38	0
2	SO4	B	1221	-	4,4,4	0.29	0	6,6,6	0.23	0
2	SO4	C	1221	-	4,4,4	0.60	0	6,6,6	1.51	1 (16%)
2	SO4	D	1221	-	4,4,4	0.56	0	6,6,6	0.71	0
2	SO4	D	1222	-	4,4,4	0.91	0	6,6,6	0.99	0
2	SO4	E	1221	-	4,4,4	0.21	0	6,6,6	0.44	0
2	SO4	F	1221	-	4,4,4	0.29	0	6,6,6	0.70	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	1221	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1221	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1221	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1221	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1222	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1221	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1221	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1221	SO4	O4-S-O3	-2.74	97.84	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1221	SO4	1	0
2	E	1221	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	93/131 (70%)	1.11	17 (18%)	2 1	23, 29, 45, 52	0
1	B	85/131 (64%)	0.78	11 (12%)	5 4	23, 28, 36, 43	0
1	C	99/131 (75%)	0.77	15 (15%)	3 2	23, 29, 44, 47	0
1	D	93/131 (70%)	0.67	12 (12%)	5 4	23, 29, 41, 49	0
1	E	99/131 (75%)	1.16	22 (22%)	1 1	23, 29, 41, 46	0
1	F	90/131 (68%)	0.89	12 (13%)	4 4	23, 29, 38, 43	0
All	All	559/786 (71%)	0.90	89 (15%)	3 2	23, 29, 42, 52	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	5.8
1	B	203	ASN	5.4
1	A	134	LYS	4.3
1	A	126	PRO	4.2
1	F	127	GLU	3.9
1	E	162	ARG	3.9
1	C	195	ILE	3.9
1	E	136	ILE	3.9
1	F	134	LYS	3.8
1	F	124	GLU	3.8
1	E	163	VAL	3.8
1	E	124	GLU	3.6
1	E	135	THR	3.6
1	A	127	GLU	3.6
1	C	158	SER	3.6
1	E	134	LYS	3.6
1	C	127	GLU	3.6
1	A	178	ILE	3.5
1	E	132	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	134	LYS	3.4
1	A	179	GLY	3.3
1	C	203	ASN	3.2
1	C	124	GLU	3.2
1	C	152	ILE	3.2
1	A	188	LEU	3.1
1	A	189	GLN	3.1
1	B	189	GLN	3.1
1	E	130	GLU	3.1
1	E	133	GLU	3.1
1	D	120	GLU	3.0
1	A	203	ASN	3.0
1	F	136	ILE	2.9
1	E	217	PHE	2.9
1	F	170	PHE	2.8
1	E	173	GLU	2.8
1	F	179	GLY	2.8
1	A	135	THR	2.7
1	B	128	ASP	2.7
1	C	136	ILE	2.7
1	A	220	THR	2.7
1	C	121	THR	2.7
1	A	151	ILE	2.6
1	D	171	CYS	2.6
1	A	152	ILE	2.6
1	D	170	PHE	2.6
1	A	170	PHE	2.6
1	E	127	GLU	2.5
1	C	128	ASP	2.5
1	D	202	LYS	2.5
1	D	133	GLU	2.5
1	E	160	GLU	2.4
1	F	203	ASN	2.4
1	F	218	ILE	2.4
1	C	153	ILE	2.4
1	E	137	ILE	2.4
1	F	171	CYS	2.4
1	E	152	ILE	2.4
1	C	178	ILE	2.4
1	E	128	ASP	2.3
1	F	153	ILE	2.3
1	B	134	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	203	ASN	2.3
1	D	153	ILE	2.3
1	E	123	PRO	2.3
1	E	156	THR	2.3
1	D	178	ILE	2.2
1	C	130	GLU	2.2
1	B	133	GLU	2.2
1	A	153	ILE	2.2
1	F	152	ILE	2.2
1	B	179	GLY	2.2
1	C	189	GLN	2.1
1	D	179	GLY	2.1
1	B	122	VAL	2.1
1	A	131	ILE	2.1
1	D	195	ILE	2.1
1	F	189	GLN	2.1
1	D	152	ILE	2.1
1	B	130	GLU	2.1
1	C	200	SER	2.1
1	D	121	THR	2.1
1	B	136	ILE	2.0
1	E	139	PRO	2.0
1	A	186	GLY	2.0
1	B	127	GLU	2.0
1	C	179	GLY	2.0
1	E	202	LYS	2.0
1	B	200	SER	2.0
1	E	220	THR	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 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
2	SO4	B	1221	5/5	0.89	0.20	0.43	99,101,101,102	0
2	SO4	A	1221	5/5	0.80	0.22	0.17	109,109,111,111	0
2	SO4	E	1221	5/5	0.66	0.19	-0.40	107,108,109,109	0
2	SO4	C	1221	5/5	0.89	0.17	-0.90	64,65,67,68	0
2	SO4	D	1222	5/5	0.94	0.16	-1.17	58,59,61,62	0
2	SO4	F	1221	5/5	0.88	0.18	-1.21	88,89,90,92	0
2	SO4	D	1221	5/5	0.92	0.13	-1.65	62,63,65,67	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.