



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

PDB ID : 1ZJ9  
Title : Structure of Mycobacterium tuberculosis NirA protein  
Authors : Schnell, R.; Sandalova, T.; Hellman, U.; Lindqvist, Y.; Schneider, G.  
Deposited on : 2005-04-28  
Resolution : 2.90 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](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

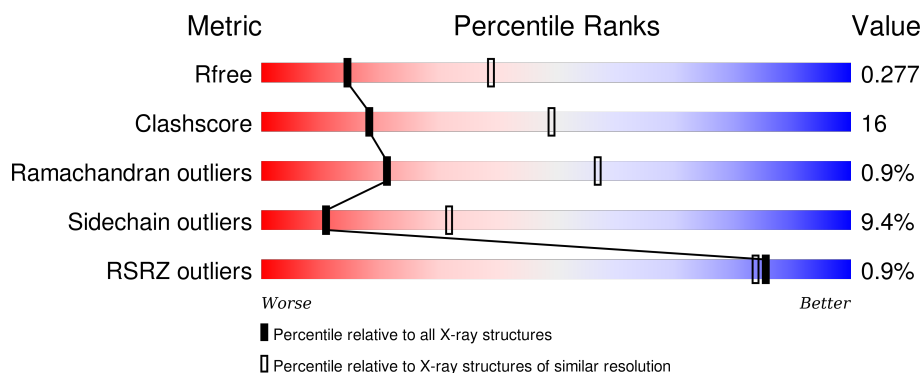
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	566	<div> <div></div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
1	B	566	<div> <div></div> <div>62%</div> <div>31%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	556	-	-	X	-
3	SF4	B	1556	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8792 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 Probable ferredoxin-dependent nitrite reductase NirA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4316	2714	792	797	13			
1	B	546	Total	C	N	O	S	0	0	0
			4316	2714	792	797	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P71753
A	-9	ASP	-	EXPRESSION TAG	UNP P71753
A	-8	VAL	-	EXPRESSION TAG	UNP P71753
A	-7	SER	-	EXPRESSION TAG	UNP P71753
A	-6	HIS	-	EXPRESSION TAG	UNP P71753
A	-5	HIS	-	EXPRESSION TAG	UNP P71753
A	-4	HIS	-	EXPRESSION TAG	UNP P71753
A	-3	HIS	-	EXPRESSION TAG	UNP P71753
A	-2	HIS	-	EXPRESSION TAG	UNP P71753
A	-1	HIS	-	EXPRESSION TAG	UNP P71753
A	0	GLY	-	EXPRESSION TAG	UNP P71753
A	1	MET	-	EXPRESSION TAG	UNP P71753
A	2	ALA	-	EXPRESSION TAG	UNP P71753
B	-10	MET	-	EXPRESSION TAG	UNP P71753
B	-9	ASP	-	EXPRESSION TAG	UNP P71753
B	-8	VAL	-	EXPRESSION TAG	UNP P71753
B	-7	SER	-	EXPRESSION TAG	UNP P71753
B	-6	HIS	-	EXPRESSION TAG	UNP P71753
B	-5	HIS	-	EXPRESSION TAG	UNP P71753
B	-4	HIS	-	EXPRESSION TAG	UNP P71753
B	-3	HIS	-	EXPRESSION TAG	UNP P71753
B	-2	HIS	-	EXPRESSION TAG	UNP P71753
B	-1	HIS	-	EXPRESSION TAG	UNP P71753
B	0	GLY	-	EXPRESSION TAG	UNP P71753
B	1	MET	-	EXPRESSION TAG	UNP P71753

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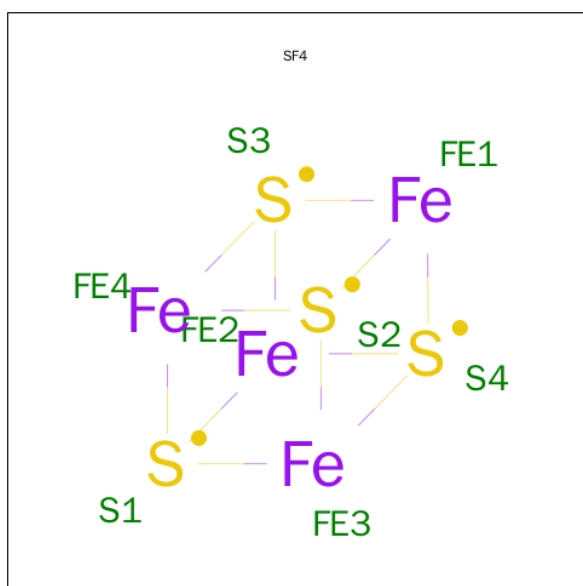
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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	EXPRESSION TAG	UNP P71753

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

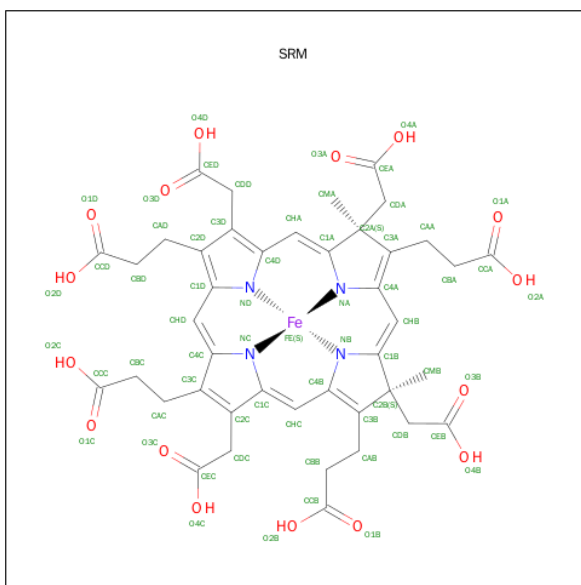
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula: C<sub>42</sub>H<sub>42</sub>FeN<sub>4</sub>O<sub>16</sub>).

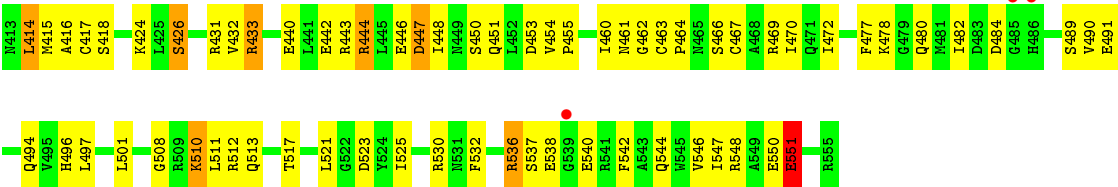


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
4	B	1	Total 63	C 42	Fe 1	N 4	O 16	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total O 13 13	0	0
5	B	3	Total O 3 3	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.98 Å   83.31 Å   108.80 Å 90.00°   102.22°   90.00°	Depositor
Resolution (Å)	55.00 – 2.90 106.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (55.00-2.90) 99.0 (106.34-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.202   ,   0.280 0.204   ,   0.277	Depositor DCC
$R_{free}$ test set	1203 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 27.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 23433 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CL, SRM

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	0.60	3/4409 (0.1%)	0.69	1/5974 (0.0%)
1	B	0.55	0/4409	0.67	0/5974
All	All	0.57	3/8818 (0.0%)	0.68	1/11948 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	GLY	C-N	17.29	1.73	1.34
1	A	100	CYS	CB-SG	-6.36	1.71	1.82
1	A	490	VAL	C-N	-5.89	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	GLY	O-C-N	-7.24	111.11	122.70

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	4316	0	4255	125	0
1	B	4316	0	4256	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	1	0
2	B	1	0	0	1	0
3	A	8	0	0	6	0
3	B	8	0	0	5	0
4	A	63	0	34	8	0
4	B	63	0	34	9	0
5	A	13	0	0	0	0
5	B	3	0	0	0	0
All	All	8792	0	8579	271	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 16.

All (271) 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:A:479:GLY:C	1:A:480:GLN:N	1.73	1.40
1:B:469:ARG:HG2	1:B:472:ILE:HD11	1.42	1.00
1:A:132:ASN:ND2	4:A:569:SRM:O1B	1.99	0.96
1:A:463:CYS:HB2	1:A:464:PRO:HD2	1.45	0.96
1:A:426:SER:CB	3:A:556:SF4:S2	2.60	0.89
1:A:426:SER:HB2	3:A:556:SF4:S2	2.12	0.89
1:A:239:LEU:HD13	1:A:266:VAL:HG21	1.54	0.88
1:B:376:THR:HG22	1:B:378:TYR:H	1.35	0.88
1:B:462:GLY:HA3	3:B:1556:SF4:S2	2.13	0.88
1:A:376:THR:HG22	1:A:378:TYR:H	1.40	0.87
1:B:431:ARG:HH11	1:B:431:ARG:HG3	1.40	0.85
1:B:207:LYS:NZ	2:B:1570:CL:CL	2.47	0.84
1:A:206:ARG:NH2	4:A:569:SRM:O4D	2.15	0.80
1:A:490:VAL:HG12	1:A:491:GLU:H	1.47	0.79
1:B:22:PRO:HG3	1:B:31:LYS:HG3	1.65	0.78
1:A:426:SER:HB3	3:A:556:SF4:S2	2.25	0.77
1:A:440:GLU:O	1:A:444:ARG:HB2	1.86	0.75
1:B:132:ASN:HD21	1:B:167:VAL:CG2	1.99	0.75
1:A:232:HIS:CD2	1:A:235:HIS:H	2.05	0.75
1:B:426:SER:HB3	3:B:1556:SF4:S2	2.27	0.74
1:B:409:HIS:ND1	1:B:455:PRO:HB3	2.03	0.74
1:A:96:MET:CE	1:A:146:ILE:HG21	2.19	0.71
1:A:96:MET:HE3	1:A:146:ILE:HG21	1.71	0.71
1:A:70:THR:HG23	1:A:424:LYS:NZ	2.06	0.71
1:A:357:ILE:O	1:A:361:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:569:SRM:HBD2	4:A:569:SRM:CED	2.22	0.70
1:B:337:LEU:HD21	1:B:343:ALA:HB2	1.73	0.70
1:B:224:ASP:OD2	1:B:290:ARG:NH2	2.24	0.70
1:B:206:ARG:HD2	1:B:289:ALA:HB3	1.74	0.70
1:B:11:ASN:OD1	1:B:19:HIS:HB3	1.91	0.69
1:A:462:GLY:HA3	3:A:556:SF4:S2	2.33	0.69
1:B:431:ARG:HG3	1:B:431:ARG:NH1	2.03	0.69
1:A:132:ASN:OD1	1:A:167:VAL:HG11	1.93	0.69
1:B:113:LEU:HD12	1:B:135:TYR:OH	1.93	0.69
1:B:30:LYS:NZ	1:B:204:LEU:O	2.26	0.69
1:B:175:GLY:HA2	1:B:183:ASP:OD2	1.92	0.69
1:B:521:LEU:O	1:B:525:ILE:HG12	1.93	0.68
1:B:34:ASN:HB3	1:B:37:ASP:OD2	1.94	0.68
1:B:132:ASN:ND2	1:B:167:VAL:HG21	2.08	0.67
1:A:232:HIS:HD2	1:A:235:HIS:H	1.41	0.67
1:A:221:GLU:HB2	1:A:501:LEU:HD22	1.75	0.67
1:B:373:ILE:HD11	1:B:381:LEU:HD12	1.76	0.67
1:B:444:ARG:HH22	1:B:523:ASP:HA	1.60	0.67
1:A:252:MET:HE1	1:A:296:LYS:HB2	1.76	0.67
1:B:417:CYS:HB2	3:B:1556:SF4:S1	2.35	0.66
1:A:463:CYS:CB	1:A:464:PRO:HD2	2.24	0.66
1:B:46:TYR:HB3	1:B:54:ILE:HG12	1.78	0.66
1:B:463:CYS:HB2	1:B:464:PRO:HD2	1.78	0.65
1:A:405:SER:C	1:A:407:PRO:HD3	2.18	0.65
1:B:544:GLN:O	1:B:547:ILE:HG13	1.97	0.65
1:B:221:GLU:HB2	1:B:501:LEU:HD22	1.78	0.64
1:B:252:MET:HE1	1:B:296:LYS:HB2	1.79	0.64
1:B:255:GLN:HB2	1:B:300:ILE:HD11	1.80	0.64
1:A:417:CYS:HB2	3:A:556:SF4:S1	2.38	0.64
1:A:203:ASP:OD1	1:A:283:ARG:NH2	2.32	0.63
1:B:132:ASN:HD21	1:B:167:VAL:HG22	1.64	0.63
1:B:38:VAL:O	1:B:42:ILE:HG12	1.99	0.62
1:A:70:THR:HG23	1:A:424:LYS:HZ1	1.64	0.62
1:B:166:ARG:NH2	1:B:207:LYS:HB3	2.13	0.62
1:B:132:ASN:HD21	1:B:167:VAL:HG21	1.65	0.62
1:A:378:TYR:O	1:A:380:LYS:HD2	1.98	0.62
1:B:470:ILE:HD13	1:B:478:LYS:HG3	1.81	0.62
1:B:111:ARG:HG2	1:B:115:GLN:NE2	2.16	0.60
1:A:105:LEU:HB2	1:A:373:ILE:HG23	1.83	0.60
1:B:164:CYS:HB2	1:B:165:PRO:CD	2.31	0.60
1:B:207:LYS:HE3	4:B:1569:SRM:O3D	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:OE2	1:A:148:ARG:NH2	2.35	0.60
1:A:64:ARG:O	1:A:161:CYS:HB2	2.01	0.59
1:B:268:GLU:OE2	1:B:314:ARG:NH2	2.27	0.59
1:B:34:ASN:OD1	1:B:35:PRO:HD2	2.03	0.59
1:B:46:TYR:CD1	1:B:54:ILE:HA	2.37	0.59
1:B:381:LEU:HD23	1:B:381:LEU:N	2.18	0.59
1:B:38:VAL:HG21	1:B:62:ARG:CB	2.33	0.59
1:A:494:GLN:HE22	1:A:510:LYS:HE3	1.66	0.59
1:A:469:ARG:HG2	1:A:472:ILE:HD11	1.85	0.58
1:B:232:HIS:HD2	1:B:234:GLU:H	1.48	0.58
1:A:392:ASP:N	1:A:392:ASP:OD1	2.36	0.58
1:B:96:MET:HE1	1:B:146:ILE:HD13	1.84	0.57
1:A:454:VAL:CG2	1:A:455:PRO:HD2	2.34	0.57
1:B:462:GLY:CA	3:B:1556:SF4:S2	2.91	0.57
1:A:513:GLN:H	1:A:555:ARG:NH2	2.03	0.57
1:B:190:GLU:O	1:B:194:ARG:HB2	2.04	0.57
1:A:532:PHE:O	1:A:536:ARG:HB3	2.05	0.57
1:B:46:TYR:CE1	1:B:54:ILE:HA	2.40	0.56
1:A:373:ILE:HD11	1:A:381:LEU:HD12	1.86	0.56
1:A:131:GLN:HG2	1:A:375:PHE:O	2.05	0.56
1:A:168:VAL:HG22	1:A:210:THR:HB	1.87	0.56
1:B:14:GLN:OE1	1:B:17:LEU:HD12	2.06	0.56
1:B:239:LEU:HD13	1:B:266:VAL:HG21	1.86	0.56
1:B:442:GLU:O	1:B:446:GLU:HB2	2.07	0.55
1:B:467:CYS:HA	4:B:1569:SRM:C4C	2.37	0.55
1:B:11:ASN:OD1	1:B:19:HIS:CB	2.54	0.55
1:B:444:ARG:NH2	1:B:523:ASP:HA	2.21	0.55
1:A:227:PHE:C	1:A:228:ILE:HD12	2.27	0.55
1:B:247:LEU:HD12	1:B:469:ARG:HG3	1.88	0.55
1:B:128:SER:OG	1:B:132:ASN:HB2	2.07	0.55
1:A:176:GLU:HB3	1:A:337:LEU:HB3	1.89	0.55
1:B:209:LYS:NZ	4:B:1569:SRM:O1C	2.33	0.54
1:A:206:ARG:HH22	4:A:569:SRM:CED	2.18	0.54
1:B:482:ILE:HD11	1:B:517:THR:HG22	1.89	0.54
4:B:1569:SRM:CED	4:B:1569:SRM:HBD2	2.38	0.54
1:A:73:GLU:HA	1:A:91:ALA:HB2	1.89	0.54
1:B:187:ALA:O	1:B:191:ILE:HG13	2.08	0.54
1:A:206:ARG:HD2	1:A:289:ALA:HB3	1.90	0.54
1:B:532:PHE:O	1:B:536:ARG:HB2	2.07	0.53
1:A:494:GLN:HE22	1:A:510:LYS:CE	2.22	0.53
1:A:247:LEU:HD12	1:A:469:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:HIS:CE1	1:B:510:LYS:HD2	2.43	0.53
1:A:490:VAL:CG1	1:A:491:GLU:H	2.19	0.53
1:A:433:ARG:NH1	1:A:518:SER:O	2.42	0.53
1:A:444:ARG:NH2	1:A:523:ASP:OD1	2.38	0.53
1:B:544:GLN:O	1:B:547:ILE:CG1	2.57	0.53
1:A:232:HIS:CD2	1:A:234:GLU:H	2.27	0.53
1:A:454:VAL:HG23	1:A:455:PRO:HD2	1.91	0.53
1:B:467:CYS:HA	4:B:1569:SRM:C3C	2.39	0.53
1:A:339:ASN:ND2	1:A:341:LEU:HD12	2.24	0.52
1:B:461:ASN:OD1	1:B:466:SER:HA	2.10	0.52
1:B:497:LEU:O	1:B:508:GLY:HA2	2.10	0.52
1:B:64:ARG:O	1:B:161:CYS:HB2	2.09	0.52
1:B:376:THR:HG22	1:B:378:TYR:N	2.14	0.52
1:A:163:ASP:HB3	1:A:204:LEU:O	2.09	0.52
1:B:511:LEU:HD22	1:B:551:GLU:OE2	2.08	0.52
1:B:447:ASP:CG	1:B:530:ARG:HH12	2.13	0.52
1:A:69:TYR:CE2	4:A:569:SRM:HMA2	2.45	0.52
1:B:38:VAL:HG21	1:B:62:ARG:HB2	1.90	0.52
1:B:127:ILE:HG22	1:B:379:GLN:HA	1.91	0.52
1:A:37:ASP:O	1:A:40:GLU:HG2	2.09	0.52
1:B:113:LEU:HG	1:B:133:VAL:HG21	1.92	0.51
1:B:41:ARG:HD2	1:B:46:TYR:OH	2.10	0.51
1:B:232:HIS:HE1	1:B:318:ASP:O	1.93	0.51
1:B:255:GLN:CB	1:B:300:ILE:HD11	2.40	0.51
1:A:513:GLN:H	1:A:555:ARG:HH22	1.57	0.51
1:A:429:GLU:HG3	1:A:433:ARG:HB2	1.92	0.51
1:B:103:GLY:HA2	1:B:131:GLN:HB3	1.92	0.51
1:A:252:MET:HE1	1:A:292:LYS:O	2.10	0.51
1:A:116:ILE:HD13	1:A:146:ILE:HG23	1.91	0.51
1:A:24:ASN:HB2	1:A:27:GLU:H	1.75	0.51
1:B:232:HIS:CD2	1:B:234:GLU:H	2.28	0.51
1:B:41:ARG:HB3	1:B:46:TYR:HE2	1.76	0.50
1:A:143:VAL:HB	1:A:144:PRO:HD3	1.93	0.50
1:A:59:LEU:CD1	1:A:94:PHE:HZ	2.24	0.50
1:B:175:GLY:CA	1:B:183:ASP:OD2	2.58	0.50
1:A:111:ARG:NH1	1:A:363:ASP:OD1	2.27	0.50
1:A:339:ASN:HB3	1:A:341:LEU:H	1.77	0.50
1:A:96:MET:HE1	1:A:146:ILE:HG21	1.92	0.50
1:B:55:ASP:N	1:B:55:ASP:OD1	2.41	0.50
1:A:239:LEU:HD13	1:A:266:VAL:CG2	2.35	0.50
1:B:41:ARG:HB3	1:B:46:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LEU:HD23	1:B:415:MET:N	2.26	0.50
1:B:38:VAL:HG21	1:B:62:ARG:HB3	1.94	0.49
1:B:13:GLY:HA2	1:B:19:HIS:HB2	1.94	0.49
1:B:35:PRO:HA	1:B:62:ARG:HD3	1.94	0.49
1:A:529:VAL:O	1:A:532:PHE:HB3	2.13	0.49
1:A:458:VAL:HA	1:A:475:ILE:O	2.13	0.49
1:B:463:CYS:HB2	1:B:464:PRO:CD	2.43	0.49
1:B:226:ALA:HB3	1:B:242:TRP:HB2	1.94	0.48
1:A:353:VAL:HG21	1:A:358:LEU:HD21	1.95	0.48
1:A:252:MET:CE	1:A:296:LYS:HB2	2.40	0.48
1:A:413:ASN:HB3	1:A:457:THR:HG22	1.96	0.48
1:B:116:ILE:HD13	1:B:146:ILE:HG23	1.95	0.48
1:B:378:TYR:O	1:B:380:LYS:HD2	2.14	0.48
1:A:436:HIS:O	1:A:439:PRO:HD2	2.14	0.48
1:A:96:MET:HE3	1:A:146:ILE:CG2	2.43	0.47
1:A:170:GLY:HA2	1:A:212:ILE:O	2.14	0.47
1:A:490:VAL:HG12	1:A:491:GLU:N	2.24	0.47
1:A:273:VAL:HG13	1:A:303:PHE:HZ	1.80	0.47
1:B:86:ILE:O	1:B:90:GLU:HB2	2.14	0.47
1:A:102:GLY:C	1:A:131:GLN:HE21	2.18	0.47
1:B:346:VAL:HG11	1:B:398:LEU:HD13	1.96	0.47
1:B:195:TYR:CZ	1:B:271:ALA:HB2	2.50	0.47
1:B:163:ASP:OD2	1:B:286:ARG:NH2	2.38	0.47
1:A:24:ASN:O	1:A:28:GLU:HB2	2.15	0.47
1:A:226:ALA:HB3	1:A:242:TRP:HB2	1.96	0.47
1:A:16:ALA:HB2	1:A:279:ASP:HB3	1.95	0.47
1:B:111:ARG:HG2	1:B:115:GLN:HE22	1.77	0.47
1:A:130:ARG:HE	1:A:167:VAL:HG23	1.80	0.46
1:A:305:GLU:O	1:A:309:THR:HG23	2.15	0.46
1:A:207:LYS:HZ1	4:A:569:SRM:C4D	2.28	0.46
1:B:432:VAL:O	1:B:433:ARG:C	2.54	0.46
1:B:232:HIS:CD2	1:B:235:HIS:H	2.33	0.46
1:A:339:ASN:CB	1:A:341:LEU:H	2.29	0.46
1:A:130:ARG:HB2	4:A:569:SRM:CBB	2.46	0.46
1:A:129:ASP:HB3	1:A:379:GLN:HG3	1.98	0.46
1:B:164:CYS:HB2	1:B:165:PRO:HD2	1.97	0.45
1:B:163:ASP:HB3	1:B:204:LEU:O	2.16	0.45
1:A:166:ARG:NH1	2:A:570:CL:CL	2.85	0.45
1:A:482:ILE:HD11	1:A:517:THR:HG22	1.99	0.45
1:A:51:PHE:CE1	1:A:92:LYS:HA	2.52	0.45
1:B:70:THR:HG22	1:B:424:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:N	1:A:89:LEU:O	2.44	0.45
1:A:220:HIS:CB	1:A:228:ILE:HD11	2.45	0.45
1:A:249:THR:HG22	1:A:464:PRO:HB2	1.99	0.45
1:A:232:HIS:HD2	1:A:234:GLU:H	1.63	0.45
1:B:145:GLU:OE2	1:B:148:ARG:NH2	2.50	0.45
1:B:469:ARG:NH1	4:B:1569:SRM:O4C	2.45	0.44
1:A:481:MET:HE2	1:A:491:GLU:HA	1.98	0.44
1:A:337:LEU:HD11	1:A:343:ALA:HB2	1.99	0.44
1:B:170:GLY:HA2	1:B:212:ILE:O	2.17	0.44
1:B:290:ARG:HD3	4:B:1569:SRM:O1D	2.17	0.44
1:B:440:GLU:HG2	1:B:444:ARG:HG3	1.98	0.44
1:A:466:SER:HA	1:A:470:ILE:HG13	1.99	0.44
1:B:42:ILE:CD1	1:B:63:PHE:CE1	3.00	0.44
1:B:350:ALA:O	1:B:431:ARG:NH1	2.50	0.44
1:B:84:ASP:N	1:B:84:ASP:OD1	2.49	0.44
1:B:95:MET:HA	1:B:135:TYR:O	2.17	0.44
1:B:431:ARG:HH11	1:B:431:ARG:CG	2.20	0.44
1:A:70:THR:HG23	1:A:424:LYS:HZ2	1.82	0.44
1:A:72:ARG:NH2	1:A:76:TYR:O	2.39	0.44
1:B:166:ARG:CZ	1:B:207:LYS:HB3	2.47	0.44
1:B:88:LYS:HA	1:B:88:LYS:HD3	1.42	0.44
1:B:426:SER:CB	3:B:1556:SF4:S2	3.02	0.43
1:B:477:PHE:CZ	1:B:525:ILE:HD11	2.53	0.43
1:B:542:PHE:O	1:B:546:VAL:HG23	2.18	0.43
1:B:182:LEU:O	1:B:214:GLY:HA3	2.18	0.43
4:B:1569:SRM:HAB1	4:B:1569:SRM:HMB3	1.83	0.43
1:A:406:ARG:N	1:A:407:PRO:HD3	2.33	0.43
1:A:454:VAL:HG21	1:A:541:ARG:HG2	2.01	0.43
1:B:416:ALA:HA	1:B:460:ILE:O	2.18	0.43
1:A:269:VAL:O	1:A:273:VAL:HG23	2.19	0.43
1:A:495:VAL:HG23	1:A:514:HIS:HD2	1.83	0.43
1:B:334:VAL:HA	1:B:343:ALA:O	2.19	0.43
1:A:404:GLN:O	1:A:407:PRO:HG3	2.19	0.43
1:B:387:PRO:HG2	1:B:390:LEU:HD12	2.01	0.43
1:B:538:GLU:CD	1:B:538:GLU:H	2.22	0.43
1:B:540:GLU:OE2	1:B:548:ARG:NH1	2.51	0.43
1:B:376:THR:HB	1:B:380:LYS:H	1.83	0.42
1:A:125:ALA:O	1:A:353:VAL:O	2.37	0.42
1:B:16:ALA:HB2	1:B:279:ASP:HB3	2.00	0.42
1:A:99:ARG:HG3	1:A:167:VAL:HG12	2.01	0.42
1:A:24:ASN:OD1	1:A:284:ARG:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASN:OD1	1:B:19:HIS:CG	2.73	0.42
1:A:337:LEU:HB2	1:A:339:ASN:HB2	2.00	0.42
1:A:461:ASN:CG	1:A:470:ILE:HG12	2.40	0.42
1:A:463:CYS:HB2	1:A:464:PRO:CD	2.30	0.42
1:B:259:ALA:HB1	1:B:316:LEU:HB3	2.02	0.42
1:A:467:CYS:HB2	3:A:556:SF4:S3	2.59	0.42
1:A:407:PRO:HB3	1:A:411:ARG:HD3	2.02	0.42
1:B:391:LEU:O	1:B:395:ILE:HG12	2.19	0.42
1:B:130:ARG:HB2	4:B:1569:SRM:CBB	2.49	0.41
1:A:131:GLN:OE1	1:A:377:PRO:HG3	2.20	0.41
1:A:352:ARG:NH1	1:A:431:ARG:HG2	2.35	0.41
1:B:409:HIS:CE1	1:B:455:PRO:HB3	2.54	0.41
1:B:206:ARG:O	1:B:207:LYS:C	2.57	0.41
1:A:497:LEU:O	1:A:508:GLY:HA2	2.20	0.41
1:B:330:ASP:OD2	1:B:412:ARG:NE	2.45	0.41
1:B:166:ARG:HH22	1:B:207:LYS:HE2	1.86	0.41
1:B:536:ARG:HG2	1:B:537:SER:N	2.36	0.41
1:B:56:LYS:HD3	1:B:60:ARG:HH21	1.86	0.41
1:B:96:MET:HE1	1:B:146:ILE:CD1	2.49	0.41
1:A:24:ASN:HD22	1:A:27:GLU:HG2	1.86	0.41
1:A:344:VAL:O	1:A:382:VAL:HA	2.20	0.41
1:A:184:PRO:HA	1:A:263:LEU:HD11	2.03	0.41
1:A:266:VAL:HB	1:A:267:PRO:HD3	2.03	0.41
1:B:454:VAL:HG22	1:B:455:PRO:HD2	2.03	0.41
1:A:51:PHE:CZ	1:A:92:LYS:HA	2.56	0.41
1:A:467:CYS:HB3	4:A:569:SRM:HDB1	2.03	0.41
1:A:232:HIS:HD2	1:A:235:HIS:N	2.13	0.41
1:A:494:GLN:NE2	1:A:510:LYS:HE3	2.33	0.41
1:A:38:VAL:O	1:A:42:ILE:HG12	2.21	0.41
1:B:433:ARG:HD3	1:B:521:LEU:HD12	2.03	0.41
1:B:46:TYR:CD1	1:B:54:ILE:HG12	2.56	0.41
1:B:470:ILE:CD1	1:B:478:LYS:HG3	2.49	0.41
1:A:494:GLN:HG2	1:A:495:VAL:N	2.36	0.41
1:B:205:PRO:HD3	1:B:283:ARG:NH1	2.35	0.41
1:B:125:ALA:O	1:B:353:VAL:O	2.39	0.41
1:B:117:SER:HB2	1:B:135:TYR:CE1	2.56	0.41
1:B:490:VAL:HG12	1:B:491:GLU:H	1.86	0.40
1:B:130:ARG:O	1:B:131:GLN:HB2	2.21	0.40
1:A:463:CYS:CB	1:A:464:PRO:CD	2.94	0.40
1:B:262:PRO:HG2	1:B:265:GLU:HB2	2.03	0.40
1:B:24:ASN:O	1:B:28:GLU:HB2	2.22	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	544/566 (96%)	501 (92%)	39 (7%)	4 (1%)	26	63
1	B	544/566 (96%)	494 (91%)	44 (8%)	6 (1%)	17	51
All	All	1088/1132 (96%)	995 (92%)	83 (8%)	10 (1%)	21	57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	248	SER
1	A	101	ASP
1	B	56	LYS
1	B	207	LYS
1	A	512	ARG
1	B	15	TRP
1	B	400	ALA
1	A	409	HIS
1	B	551	GLU

### 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	450/465 (97%)	408 (91%)	42 (9%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	450/465 (97%)	407 (90%)	43 (10%)	10	31
All	All	900/930 (97%)	815 (91%)	85 (9%)	11	32

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	38	VAL
1	A	39	ARG
1	A	40	GLU
1	A	42	ILE
1	A	70	THR
1	A	84	ASP
1	A	86	ILE
1	A	87	ASP
1	A	113	LEU
1	A	123	ASP
1	A	138	ILE
1	A	153	VAL
1	A	167	VAL
1	A	200	ASP
1	A	206	ARG
1	A	300	ILE
1	A	305	GLU
1	A	325	VAL
1	A	326	LYS
1	A	382	VAL
1	A	385	ASP
1	A	392	ASP
1	A	393	ASP
1	A	399	ASP
1	A	433	ARG
1	A	444	ARG
1	A	446	GLU
1	A	447	ASP
1	A	456	ILE
1	A	480	GLN
1	A	484	ASP
1	A	486	HIS
1	A	489	SER
1	A	495	VAL
1	A	519	ASP

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Mol	Chain	Res	Type
1	A	534	LYS
1	A	536	ARG
1	A	538	GLU
1	A	547	ILE
1	A	552	ASP
1	A	555	ARG
1	B	11	ASN
1	B	19	HIS
1	B	55	ASP
1	B	57	THR
1	B	84	ASP
1	B	86	ILE
1	B	113	LEU
1	B	115	GLN
1	B	133	VAL
1	B	153	VAL
1	B	171	SER
1	B	207	LYS
1	B	218	VAL
1	B	247	LEU
1	B	249	THR
1	B	323	GLU
1	B	325	VAL
1	B	326	LYS
1	B	374	ARG
1	B	381	LEU
1	B	385	ASP
1	B	395	ILE
1	B	414	LEU
1	B	418	SER
1	B	426	SER
1	B	433	ARG
1	B	443	ARG
1	B	444	ARG
1	B	447	ASP
1	B	448	ILE
1	B	450	SER
1	B	451	GLN
1	B	453	ASP
1	B	480	GLN
1	B	484	ASP
1	B	489	SER

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Mol	Chain	Res	Type
1	B	494	GLN
1	B	510	LYS
1	B	512	ARG
1	B	513	GLN
1	B	536	ARG
1	B	550	GLU
1	B	551	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	131	GLN
1	A	220	HIS
1	A	232	HIS
1	A	235	HIS
1	A	480	GLN
1	A	486	HIS
1	A	494	GLN
1	A	514	HIS
1	B	115	GLN
1	B	220	HIS
1	B	232	HIS
1	B	235	HIS
1	B	496	HIS
1	B	531	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	SF4	A	556	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SRM	A	569	-	29,70,70	1.63	7 (24%)	29,112,112	3.78	19 (65%)
3	SF4	B	1556	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SRM	B	1569	-	29,70,70	1.55	6 (20%)	29,112,112	4.06	16 (55%)

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	SF4	A	556	1	-	0/0/48/48	0/6/5/5
4	SRM	A	569	-	-	0/22/126/126	0/0/8/8
3	SF4	B	1556	1	-	0/0/48/48	0/6/5/5
4	SRM	B	1569	-	-	0/22/126/126	0/0/8/8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	569	SRM	CDB-C2B	-4.22	1.49	1.56
4	B	1569	SRM	CDB-C2B	-3.94	1.50	1.56
4	B	1569	SRM	C1B-NB	-3.67	1.32	1.38
4	A	569	SRM	CDA-C2A	-3.51	1.50	1.56
4	B	1569	SRM	CDA-C2A	-3.12	1.51	1.56
4	A	569	SRM	C4B-NB	-2.95	1.33	1.39
4	A	569	SRM	C1B-NB	-2.80	1.33	1.38
4	A	569	SRM	C4A-NA	-2.65	1.34	1.39
4	B	1569	SRM	C1A-NA	-2.64	1.34	1.38
4	A	569	SRM	CDC-C2C	-2.26	1.49	1.52
4	B	1569	SRM	C4A-NA	-2.24	1.34	1.39
4	B	1569	SRM	C4B-NB	-2.07	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	569	SRM	CMA-C2A	-2.02	1.50	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1569	SRM	CAB-C3B-C2B	-12.01	109.93	123.46
4	A	569	SRM	CAB-C3B-C2B	-11.07	111.00	123.46
4	A	569	SRM	CAA-C3A-C2A	-7.95	114.52	123.46
4	B	1569	SRM	CAA-C3A-C2A	-7.59	114.91	123.46
4	B	1569	SRM	CAC-C3C-C2C	-5.43	115.86	129.38
4	A	569	SRM	CAC-C3C-C2C	-4.21	118.91	129.38
4	A	569	SRM	CAD-C2D-C1D	-3.95	122.72	127.01
4	A	569	SRM	C4B-NB-C1B	-3.85	104.81	106.90
4	B	1569	SRM	CAD-C2D-C1D	-3.81	122.87	127.01
4	B	1569	SRM	C4B-NB-C1B	-3.50	105.00	106.90
4	A	569	SRM	C4A-NA-C1A	-2.77	105.40	106.90
4	B	1569	SRM	CAC-CBC-CCC	-2.30	108.52	112.75
4	A	569	SRM	CAD-C2D-C3D	-2.27	123.75	129.38
4	A	569	SRM	CDD-C3D-C4D	-2.22	123.74	127.34
4	A	569	SRM	CAC-CBC-CCC	-2.15	108.80	112.75
4	B	1569	SRM	CAD-C2D-C3D	-2.00	124.40	129.38
4	A	569	SRM	C3B-C4B-NB	2.44	112.80	110.09
4	A	569	SRM	CEC-CDC-C2C	2.65	121.37	116.31
4	A	569	SRM	C2A-CDA-CEA	2.74	119.70	115.45
4	B	1569	SRM	C3A-C4A-NA	3.00	113.42	110.09
4	A	569	SRM	C3A-C4A-NA	3.10	113.54	110.09
4	B	1569	SRM	C3B-C4B-NB	3.21	113.66	110.09
4	A	569	SRM	CBD-CAD-C2D	3.38	118.58	112.53
4	B	1569	SRM	CED-CDD-C3D	3.50	122.99	116.31
4	A	569	SRM	CED-CDD-C3D	3.52	123.04	116.31
4	A	569	SRM	CMA-C2A-CDA	3.64	114.10	109.76
4	B	1569	SRM	CMA-C2A-CDA	4.00	114.52	109.76
4	B	1569	SRM	CBC-CAC-C3C	4.35	120.32	112.53
4	A	569	SRM	CBC-CAC-C3C	4.37	120.36	112.53
4	B	1569	SRM	CBD-CAD-C2D	4.44	120.48	112.53
4	A	569	SRM	CAC-C3C-C4C	5.10	132.55	127.01
4	B	1569	SRM	C2A-CDA-CEA	5.30	123.67	115.45
4	B	1569	SRM	CAD-CBD-CCD	5.37	122.59	112.75
4	A	569	SRM	CAD-CBD-CCD	5.70	123.19	112.75
4	B	1569	SRM	CAC-C3C-C4C	7.21	134.83	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	SF4	6	0
4	A	569	SRM	8	0
3	B	1556	SF4	5	0
4	B	1569	SRM	9	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	546/566 (96%)	-0.40	6 (1%) 82 80	18, 33, 54, 72	0
1	B	546/566 (96%)	-0.35	4 (0%) 89 88	19, 34, 55, 72	0
All	All	1092/1132 (96%)	-0.37	10 (0%) 85 84	18, 33, 54, 72	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	4.8
1	A	488	GLY	4.7
1	B	485	GLY	4.1
1	B	486	HIS	3.9
1	A	484	ASP	3.6
1	A	487	GLY	3.5
1	A	512	ARG	2.5
1	B	539	GLY	2.0
1	B	40	GLU	2.0
1	A	480	GLN	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
4	SRM	A	569	63/63	0.94	0.18	0.96	28,36,42,47	0
4	SRM	B	1569	63/63	0.94	0.17	0.92	28,34,42,46	0
3	SF4	B	1556	8/8	0.99	0.10	-1.52	24,27,28,29	0
3	SF4	A	556	8/8	0.99	0.09	-1.72	19,20,23,23	0
2	CL	B	1570	1/1	0.94	0.18	-	32,32,32,32	0
2	CL	A	570	1/1	0.80	0.30	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.