



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:36 PM GMT

PDB ID : 3ZYY  
Title : Reductive activator for corrinoid,iron-sulfur protein  
Authors : Hennig, S.E.; Jeoung, J.-H.; Goetzl, S.; Dobbek, H.  
Deposited on : 2011-08-30  
Resolution : 2.20 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

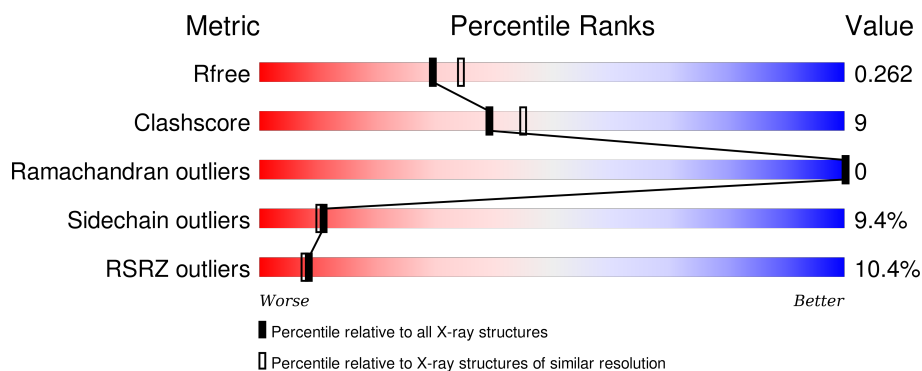
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	X	631	<div> <div>13%</div> <div>74%</div> <div>21%</div> <div>.</div> </div>
1	Y	631	<div> <div>6%</div> <div>63%</div> <div>17%</div> <div>.</div> <div>17%</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
2	FES	X	800	-	-	X	-
5	SO4	X	1631	-	-	-	X
5	SO4	X	1632	-	-	-	X
5	SO4	X	1633	-	-	-	X
5	SO4	Y	1631	-	-	-	X
6	BU3	X	1638	-	-	-	X

## 2 Entry composition [i](#)

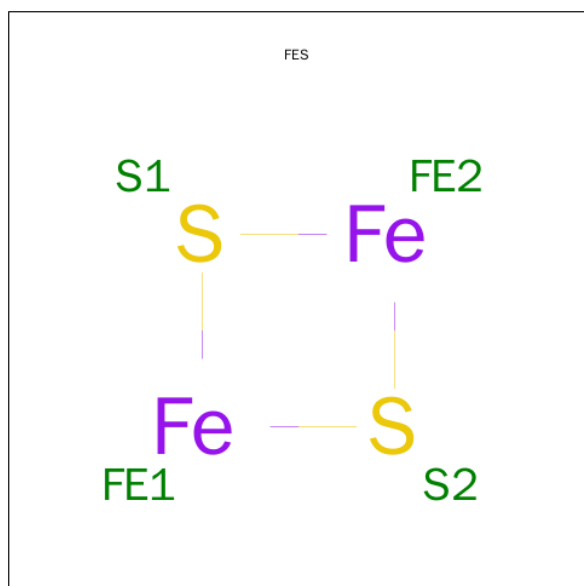
There are 7 unique types of molecules in this entry. The entry contains 9313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IRON-SULFUR CLUSTER BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	628	Total	C	N	O	S	0	7	0
			4843	3072	816	932	23			
1	Y	522	Total	C	N	O	S	0	2	0
			3995	2540	669	769	17			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	P	0	0
			5	4	1		
3	Y	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

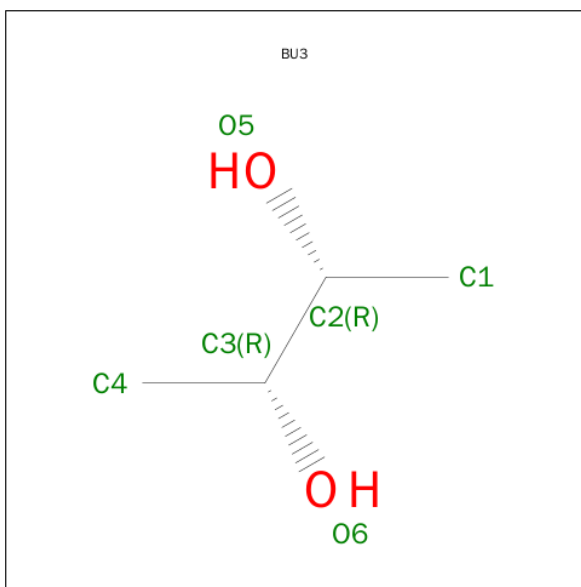
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	Mg	0	0
			1	1		
4	Y	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	X	1	Total	O	S	0	0
			5	4	1		
5	X	1	Total	O	S	0	0
			5	4	1		
5	X	1	Total	O	S	0	0
			5	4	1		
5	X	1	Total	O	S	0	0
			5	4	1		
5	X	1	Total	O	S	0	0
			5	4	1		
5	Y	1	Total	O	S	0	0
			5	4	1		
5	Y	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	X	1	Total	C	O	0	0
			6	4	2		
6	Y	1	Total	C	O	0	0
			6	4	2		
6	Y	1	Total	C	O	0	0
			6	4	2		

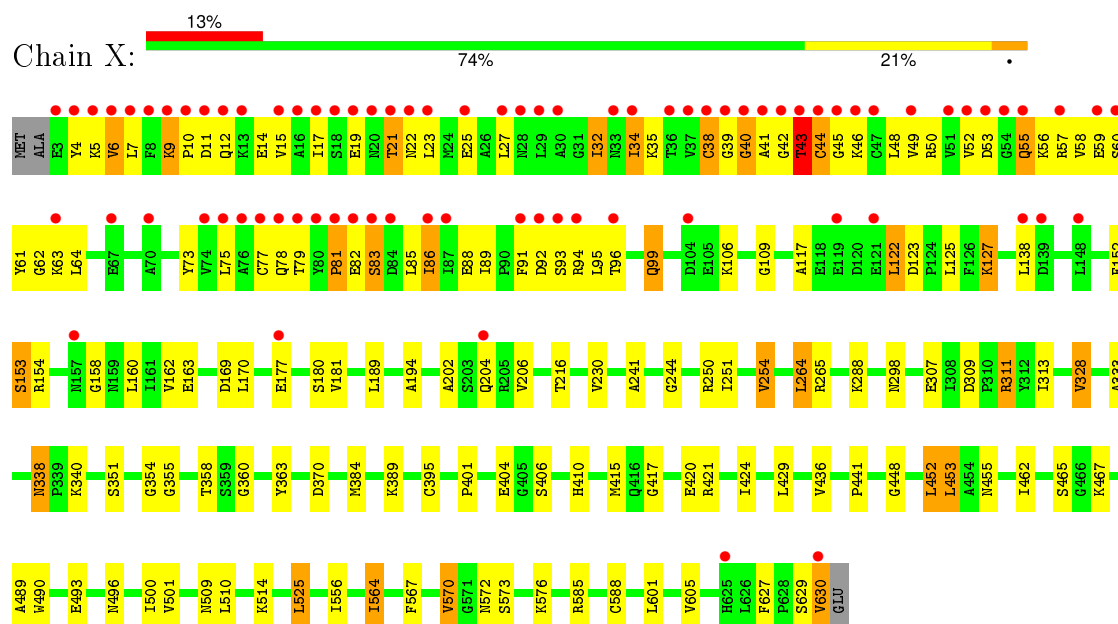
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	X	290	Total	O	0	0
			290	290		
7	Y	106	Total	O	0	0
			106	106		

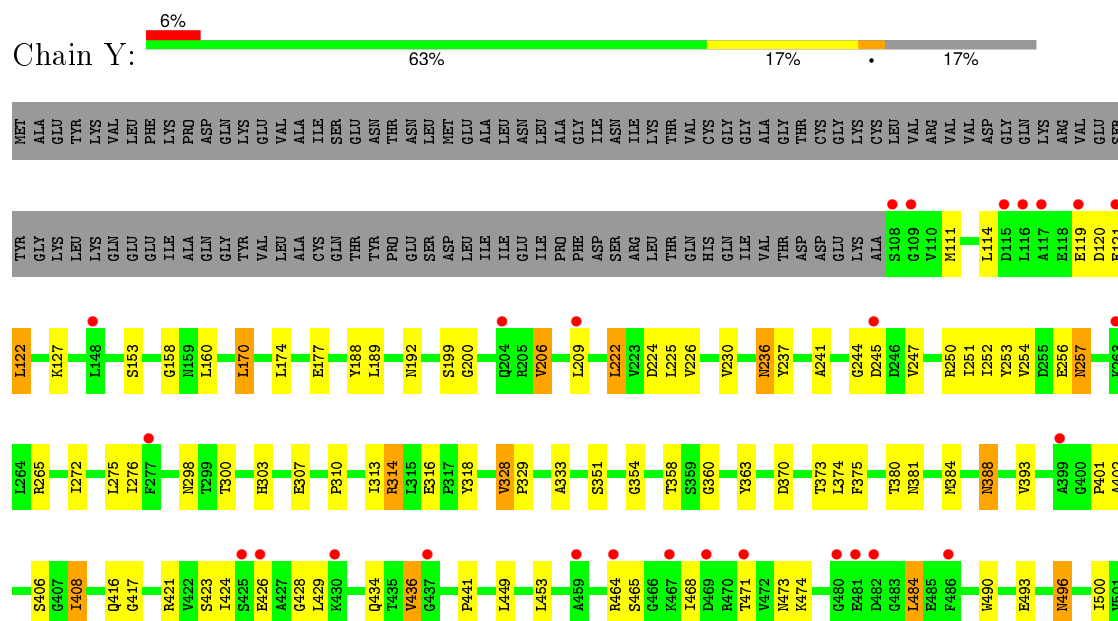
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

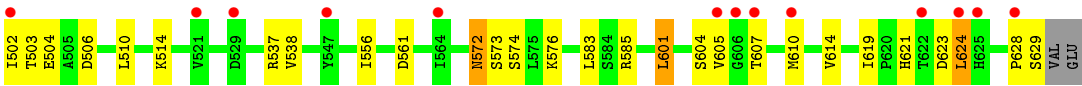
#### • Molecule 1: IRON-SULFUR CLUSTER BINDING PROTEIN



#### • Molecule 1: IRON-SULFUR CLUSTER BINDING PROTEIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.53Å 91.19Å 252.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.20 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.94-2.20) 99.8 (19.94-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, $R_{free}$	0.220 , 0.258 0.220 , 0.262	Depositor DCC
$R_{free}$ test set	4175 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 83472 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, BU3, MG, PO4, FES

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	X	0.27	1/4936 (0.0%)	0.48	0/6678
1	Y	0.23	0/4063	0.43	0/5501
All	All	0.26	1/8999 (0.0%)	0.46	0/12179

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	X	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	44	CYS	CB-SG	5.10	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	40	GLY	Peptide
1	X	43	THR	Peptide
1	X	81	PRO	Peptide
1	X	83	SER	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	X	4843	0	4948	95	0
1	Y	3995	0	4074	64	0
2	X	4	0	0	2	0
3	X	5	0	0	0	0
3	Y	5	0	0	0	0
4	X	1	0	0	0	0
4	Y	1	0	0	0	0
5	X	35	0	0	0	0
5	Y	10	0	0	0	0
6	X	6	0	10	0	0
6	Y	12	0	20	0	0
7	X	290	0	0	2	0
7	Y	106	0	0	0	0
All	All	9313	0	9052	159	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 9.

All (159) 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:X:43:THR:HB	1:X:44:CYS:HA	1.38	1.05
1:Y:496:ASN:HD22	1:Y:496:ASN:H	1.21	0.88
1:X:38:CYS:HB2	1:X:40:GLY:H	1.43	0.84
1:X:265:ARG:HD2	1:X:307:GLU:HB2	1.62	0.80
1:Y:265:ARG:HD2	1:Y:307:GLU:HB2	1.62	0.80
1:Y:236:ASN:HD22	1:Y:237:TYR:H	1.27	0.79
1:X:48:LEU:HD11	1:X:64:LEU:HD21	1.68	0.76
1:Y:313:ILE:HG23	1:Y:351:SER:HB3	1.73	0.71
1:X:43:THR:HB	1:X:44:CYS:CA	2.19	0.70
1:X:43:THR:O	1:X:75:LEU:HD11	1.92	0.70
1:X:6:VAL:HG23	1:X:15:VAL:HG23	1.73	0.70
1:X:338:ASN:HD22	1:X:340:LYS:H	1.40	0.68
1:Y:449:LEU:HD13	1:Y:510:LEU:HD21	1.76	0.67
1:X:202:ALA:HB3	1:X:204:GLN:HE21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:109:GLY:HA2	1:X:564:ILE:HD13	1.79	0.65
1:X:360:GLY:HA2	1:X:573:SER:HB2	1.78	0.64
1:X:152:PHE:CD1	1:X:160:LEU:HB2	2.34	0.63
1:X:313:ILE:HG23	1:X:351:SER:HB3	1.78	0.63
1:X:22:ASN:HB2	1:X:25:GLU:HG3	1.80	0.63
1:X:95:LEU:HD13	1:X:99:GLN:HG3	1.81	0.62
1:X:410:HIS:CD2	1:X:501:VAL:H	2.17	0.62
1:X:309:ASP:OD1	1:X:311:ARG:HD3	2.00	0.62
1:Y:177:GLU:HG3	1:Y:200:GLY:N	2.14	0.62
1:X:82:GLU:O	1:X:83:SER:HB2	2.00	0.62
1:Y:192:ASN:ND2	1:Y:585:ARG:HH12	1.98	0.61
1:X:106:LYS:HA	1:X:564:ILE:HD11	1.80	0.61
1:Y:624:LEU:HD12	1:Y:624:LEU:H	1.65	0.60
1:X:9:LYS:O	1:X:88:GLU:HA	2.02	0.60
1:X:424:ILE:H	1:X:455:ASN:ND2	2.00	0.59
1:Y:236:ASN:HD22	1:Y:237:TYR:N	1.99	0.59
1:X:424:ILE:H	1:X:455:ASN:HD22	1.51	0.59
1:Y:236:ASN:ND2	1:Y:237:TYR:H	2.00	0.58
1:X:55:GLN:H	1:X:83:SER:CB	2.17	0.58
1:X:160:LEU:HD11	1:X:194:ALA:HB2	1.88	0.56
1:X:91:PHE:O	1:X:92:ASP:HB2	2.05	0.55
1:X:250:ARG:O	1:X:254:VAL:HG13	2.07	0.55
1:X:81:PRO:HB3	1:X:85:LEU:HD22	1.89	0.55
1:Y:408:ILE:HD13	1:Y:506:ASP:HB3	1.88	0.55
1:Y:206:VAL:HG22	1:Y:225:LEU:HB2	1.88	0.54
1:Y:250:ARG:O	1:Y:254:VAL:HG12	2.08	0.54
1:Y:241:ALA:HA	1:Y:244:GLY:O	2.07	0.54
1:Y:621:HIS:CD2	1:Y:623:ASP:H	2.25	0.54
1:Y:170:LEU:HD22	1:Y:174:LEU:HD13	1.90	0.54
1:X:75:LEU:O	1:X:79:THR:HG22	2.08	0.54
1:X:45:GLY:O	1:X:48:LEU:HB2	2.09	0.52
1:X:421[A]:ARG:HG2	1:X:421[A]:ARG:HH11	1.73	0.52
1:Y:610:MET:O	1:Y:614:VAL:HG23	2.10	0.52
1:Y:621:HIS:HD2	1:Y:623:ASP:H	1.57	0.52
1:Y:363:TYR:CZ	1:Y:576:LYS:HD3	2.44	0.51
1:X:23:LEU:HD22	1:X:79:THR:CG2	2.39	0.51
1:X:60:SER:C	1:X:62:GLY:N	2.62	0.51
1:X:127:LYS:HD2	7:X:2040:HOH:O	2.10	0.51
1:X:39:GLY:N	2:X:800:FES:S1	2.66	0.51
1:X:61:TYR:O	1:X:64:LEU:HB2	2.10	0.51
1:Y:380:THR:HG23	1:Y:401:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:251:ILE:HG21	1:Y:314:ARG:HG2	1.93	0.51
1:Y:421:ARG:HB2	1:Y:434:GLN:HB2	1.92	0.50
1:X:490:TRP:O	1:X:493:GLU:HG2	2.10	0.50
1:Y:177:GLU:HG3	1:Y:200:GLY:CA	2.41	0.50
1:Y:429:LEU:HA	1:Y:473:ASN:HD22	1.75	0.50
1:X:370:ASP:OD1	1:X:389:LYS:HD3	2.12	0.50
1:X:629:SER:O	1:X:630:VAL:C	2.50	0.50
1:Y:122:LEU:HD21	1:Y:583:LEU:HD22	1.93	0.50
1:X:32:ILE:HD12	1:X:89:ILE:HD11	1.93	0.49
1:X:50:ARG:HH12	1:X:52:VAL:HA	1.78	0.49
1:X:27:LEU:HD13	1:X:34:ILE:HG23	1.94	0.49
1:X:125:LEU:HD21	1:X:588:CYS:SG	2.52	0.49
1:X:35:LYS:HE3	1:X:46:LYS:NZ	2.28	0.49
1:X:77:CYS:SG	1:X:78:GLN:HG2	2.52	0.48
1:X:23:LEU:HD22	1:X:79:THR:HG21	1.95	0.48
1:X:55:GLN:H	1:X:83:SER:HB2	1.79	0.48
1:X:355:GLY:HA2	1:X:358:THR:HG22	1.94	0.48
1:Y:253:TYR:O	1:Y:257:ASN:HB2	2.14	0.48
1:Y:360:GLY:HA2	1:Y:573:SER:HB2	1.96	0.48
1:Y:254:VAL:HG11	1:Y:310:PRO:HG3	1.95	0.48
1:X:363:TYR:HE2	1:X:570:VAL:HG22	1.79	0.48
1:X:4:TYR:CE2	1:X:82:GLU:HA	2.49	0.47
1:X:7:LEU:HB3	1:X:86:ILE:HG23	1.96	0.47
1:X:395[A]:CYS:SG	1:X:601:LEU:HB2	2.54	0.47
1:X:401:PRO:HB2	1:X:404:GLU:HB2	1.97	0.47
1:X:5:LYS:HG2	1:X:14:GLU:OE2	2.14	0.47
1:Y:572:ASN:HD21	1:Y:574:SER:HB3	1.78	0.47
1:Y:374:LEU:HB3	1:Y:538:VAL:HG22	1.97	0.47
1:X:420:GLU:C	1:X:421[B]:ARG:HG2	2.36	0.46
1:X:525:LEU:HD12	1:X:525:LEU:HA	1.74	0.46
1:X:572:ASN:O	1:X:576:LYS:HG3	2.15	0.46
1:X:123:ASP:OD2	1:X:585[A]:ARG:HD3	2.15	0.46
1:Y:328:VAL:HG22	1:Y:333:ALA:HB2	1.97	0.46
1:X:384:MET:HB2	1:X:395[B]:CYS:SG	2.56	0.46
1:X:153:SER:HA	1:X:158:GLY:O	2.16	0.46
1:X:298:ASN:HA	1:X:354:GLY:HA3	1.98	0.46
1:X:12:GLN:HB3	1:X:12:GLN:HE21	1.61	0.46
1:X:40:GLY:HA2	1:X:41:ALA:C	2.35	0.46
1:Y:401:PRO:HB2	1:Y:406:SER:HB3	1.98	0.46
1:Y:441:PRO:O	1:Y:500:ILE:HD11	2.16	0.45
1:X:564:ILE:HA	1:X:567:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:177:GLU:HG2	1:X:180:SER:HB3	1.98	0.45
1:X:448:GLY:O	1:X:452:LEU:HB2	2.17	0.45
1:X:6:VAL:CG1	1:X:85:LEU:HB3	2.47	0.45
1:Y:272:ILE:O	1:Y:276:ILE:HG13	2.16	0.45
1:Y:416:GLN:HA	1:Y:436:VAL:HG22	1.99	0.45
1:Y:496:ASN:ND2	1:Y:496:ASN:H	2.01	0.45
1:X:415:MET:O	1:X:436:VAL:HB	2.17	0.45
1:Y:236:ASN:HB2	1:Y:275:LEU:HD21	1.98	0.45
1:Y:252:ILE:O	1:Y:256[A]:GLU:HG2	2.16	0.45
1:Y:373:THR:CG2	1:Y:537:ARG:HE	2.30	0.45
1:X:10:PRO:O	1:X:94:ARG:NH2	2.50	0.44
1:Y:363:TYR:CE1	1:Y:576:LYS:HB3	2.51	0.44
1:X:401:PRO:HG2	1:X:406:SER:HB3	1.99	0.44
1:Y:247:VAL:HG13	1:Y:300:THR:HG21	2.00	0.44
1:X:328:VAL:HG22	1:X:333:ALA:HB2	1.99	0.44
1:X:424:ILE:HB	1:X:455:ASN:HB3	2.00	0.44
1:Y:484:LEU:O	1:Y:504:GLU:HG3	2.17	0.44
1:Y:556:ILE:HA	1:Y:619:ILE:HG23	2.00	0.44
1:X:241:ALA:HA	1:X:244:GLY:O	2.18	0.44
1:X:44:CYS:SG	1:X:45:GLY:N	2.91	0.44
1:Y:153:SER:HA	1:Y:158:GLY:O	2.18	0.43
1:Y:224:ASP:OD1	1:Y:226:VAL:HG12	2.18	0.43
1:Y:375:PHE:O	1:Y:384:MET:HA	2.18	0.43
1:X:355:GLY:O	1:X:358:THR:HG22	2.18	0.43
1:Y:328:VAL:HA	1:Y:329:PRO:HD3	1.91	0.43
1:Y:298:ASN:HA	1:Y:354:GLY:HA3	2.00	0.43
1:X:59:GLU:O	1:X:60:SER:HB3	2.19	0.43
1:X:163:GLU:HB3	7:X:2067:HOH:O	2.18	0.43
1:Y:402:ALA:HB1	1:Y:510:LEU:HD23	2.01	0.43
1:X:254:VAL:HG12	1:X:264:LEU:HD13	2.01	0.43
1:Y:188:TYR:CE1	1:Y:189:LEU:HD23	2.54	0.43
1:X:10:PRO:HA	1:X:11:ASP:HA	1.53	0.43
1:X:17:ILE:HG13	1:X:21:THR:OG1	2.18	0.43
1:X:40:GLY:CA	1:X:41:ALA:C	2.88	0.42
1:Y:417:GLY:O	1:Y:441:PRO:HA	2.20	0.42
1:Y:484:LEU:HB2	1:Y:504:GLU:CD	2.40	0.42
1:Y:468:ILE:HG13	1:Y:504:GLU:HG2	2.01	0.42
1:Y:316:GLU:HA	1:Y:318:TYR:H	1.85	0.42
1:X:251:ILE:O	1:X:254:VAL:HG22	2.20	0.42
1:X:489:ALA:HB3	1:X:500:ILE:HB	2.01	0.42
1:Y:192:ASN:HD21	1:Y:585:ARG:HH12	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:49:VAL:O	1:X:73:TYR:HA	2.20	0.41
1:X:99:GLN:OE1	1:X:117:ALA:HB2	2.20	0.41
1:Y:490:TRP:HB2	1:Y:493:GLU:HG3	2.01	0.41
1:Y:177:GLU:HG2	1:Y:199:SER:HB3	2.02	0.41
1:X:89:ILE:HG21	1:X:94:ARG:HE	1.84	0.41
1:Y:424:ILE:HG22	1:Y:428:GLY:HA2	2.02	0.41
1:X:60:SER:C	1:X:62:GLY:H	2.24	0.41
1:X:122:LEU:HD12	1:X:122:LEU:HA	1.91	0.41
1:X:360:GLY:CA	1:X:573:SER:HB2	2.49	0.41
1:X:216:THR:HB	1:X:404:GLU:OE1	2.21	0.41
1:Y:496:ASN:HD22	1:Y:496:ASN:N	1.98	0.41
1:Y:388:ASN:HD22	1:Y:388:ASN:N	2.19	0.41
1:X:417:GLY:O	1:X:441:PRO:HA	2.21	0.41
1:Y:561:ASP:OD2	1:Y:628:PRO:HD2	2.21	0.40
1:X:627:PHE:O	1:X:630:VAL:HG13	2.21	0.40
1:X:453:LEU:HB3	1:X:556:ILE:HG21	2.03	0.40
1:X:154:ARG:HB3	1:X:154:ARG:HE	1.78	0.40
1:Y:303:HIS:CD2	1:Y:313:ILE:HD11	2.57	0.40
1:X:462:ILE:HA	1:X:467:LYS:O	2.22	0.40
1:Y:393:VAL:HG11	1:Y:601:LEU:HD12	2.04	0.40
1:X:42:GLY:HA2	2:X:800:FES:S2	2.61	0.40
1:Y:209:LEU:HD23	1:Y:222:LEU:HD23	2.04	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	X	633/631 (100%)	613 (97%)	20 (3%)	0	100	100
1	Y	522/631 (83%)	508 (97%)	14 (3%)	0	100	100
All	All	1155/1262 (92%)	1121 (97%)	34 (3%)	0	100	100



There are no Ramachandran outliers to report.

### 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	X	531/526 (101%)	483 (91%)	48 (9%)	12	11
1	Y	435/526 (83%)	393 (90%)	42 (10%)	10	9
All	All	966/1052 (92%)	876 (91%)	90 (9%)	11	10

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	6	VAL
1	X	9	LYS
1	X	19	GLU
1	X	21	THR
1	X	32	ILE
1	X	34	ILE
1	X	38	CYS
1	X	43	THR
1	X	53	ASP
1	X	55	GLN
1	X	56	LYS
1	X	57	ARG
1	X	58	VAL
1	X	63	LYS
1	X	86	ILE
1	X	93	SER
1	X	96	THR
1	X	99	GLN
1	X	122	LEU
1	X	127	LYS
1	X	138	LEU
1	X	153	SER
1	X	162	VAL
1	X	169	ASP
1	X	170	LEU

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Mol	Chain	Res	Type
1	X	181	VAL
1	X	189	LEU
1	X	206	VAL
1	X	230	VAL
1	X	254	VAL
1	X	264	LEU
1	X	288	LYS
1	X	311	ARG
1	X	328	VAL
1	X	338	ASN
1	X	429	LEU
1	X	452	LEU
1	X	453	LEU
1	X	465	SER
1	X	496	ASN
1	X	509	ASN
1	X	510	LEU
1	X	514	LYS
1	X	525	LEU
1	X	564	ILE
1	X	570	VAL
1	X	605	VAL
1	X	630	VAL
1	Y	111	MET
1	Y	114	LEU
1	Y	119	GLU
1	Y	120	ASP
1	Y	121	GLU
1	Y	122	LEU
1	Y	127	LYS
1	Y	160	LEU
1	Y	170	LEU
1	Y	206	VAL
1	Y	222	LEU
1	Y	230	VAL
1	Y	236	ASN
1	Y	245	ASP
1	Y	257	ASN
1	Y	314	ARG
1	Y	328	VAL
1	Y	358	THR
1	Y	370	ASP

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Mol	Chain	Res	Type
1	Y	381	ASN
1	Y	388	ASN
1	Y	408	ILE
1	Y	423	SER
1	Y	426	GLU
1	Y	436	VAL
1	Y	453	LEU
1	Y	464	ARG
1	Y	465	SER
1	Y	471	THR
1	Y	474	LYS
1	Y	484	LEU
1	Y	496	ASN
1	Y	502	ILE
1	Y	503	THR
1	Y	514	LYS
1	Y	572	ASN
1	Y	601	LEU
1	Y	604	SER
1	Y	605	VAL
1	Y	607	THR
1	Y	624	LEU
1	Y	629	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	12	GLN
1	X	155	GLN
1	X	172	GLN
1	X	176	ASN
1	X	204	GLN
1	X	278	GLN
1	X	338	ASN
1	X	410	HIS
1	X	455	ASN
1	X	496	ASN
1	X	497	ASN
1	Y	112	ASN
1	Y	159	ASN
1	Y	172	GLN
1	Y	176	ASN

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Mol	Chain	Res	Type
1	Y	192	ASN
1	Y	236	ASN
1	Y	240	GLN
1	Y	257	ASN
1	Y	388	ASN
1	Y	410	HIS
1	Y	496	ASN
1	Y	572	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](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z  > 2$
5	SO4	X	1631	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	X	1632	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	X	1633	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	X	1634	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	X	1635	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	X	1636	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	X	1637	-	4,4,4	0.23	0	6,6,6	0.07	0
6	BU3	X	1638	-	4,5,5	1.60	1 (25%)	6,6,6	0.33	0
2	FES	X	800	1	0,4,4	0.00	-	0,4,4	0.00	-
3	PO4	X	801	4	4,4,4	0.51	0	6,6,6	0.27	0
5	SO4	Y	1630	-	4,4,4	0.25	0	6,6,6	0.07	0
5	SO4	Y	1631	-	4,4,4	0.24	0	6,6,6	0.09	0
6	BU3	Y	1632	-	4,5,5	1.61	1 (25%)	6,6,6	0.35	0
6	BU3	Y	1633	-	4,5,5	1.59	1 (25%)	6,6,6	0.33	0
3	PO4	Y	801	4	4,4,4	0.52	0	6,6,6	0.27	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
5	SO4	X	1631	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1632	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1633	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1634	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1635	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1636	-	-	0/0/0/0	0/0/0/0
5	SO4	X	1637	-	-	0/0/0/0	0/0/0/0
6	BU3	X	1638	-	-	0/4/4/4	0/0/0/0
2	FES	X	800	1	-	0/0/4/4	0/1/1/1
3	PO4	X	801	4	-	0/0/0/0	0/0/0/0
5	SO4	Y	1630	-	-	0/0/0/0	0/0/0/0
5	SO4	Y	1631	-	-	0/0/0/0	0/0/0/0
6	BU3	Y	1632	-	-	0/4/4/4	0/0/0/0
6	BU3	Y	1633	-	-	0/4/4/4	0/0/0/0
3	PO4	Y	801	4	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	1632	BU3	O6-C3	-2.46	1.37	1.43
6	Y	1633	BU3	O6-C3	-2.43	1.37	1.43
6	X	1638	BU3	O6-C3	-2.42	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	800	FES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	X	628/631 (99%)	0.67	80 (12%) <b>5</b> <b>4</b>	26, 43, 117, 131	22 (3%)
1	Y	522/631 (82%)	0.54	40 (7%) <b>16</b> <b>16</b>	34, 61, 89, 102	0
All	All	1150/1262 (91%)	0.61	120 (10%) <b>8</b> <b>8</b>	26, 50, 110, 131	22 (1%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	44	CYS	17.6
1	X	45	GLY	15.1
1	X	43	THR	14.7
1	X	41	ALA	13.5
1	X	42	GLY	13.4
1	X	8	PHE	10.5
1	X	39	GLY	10.3
1	X	38	CYS	9.5
1	Y	108	SER	8.6
1	X	82	GLU	8.2
1	X	49	VAL	7.9
1	X	23	LEU	7.7
1	X	4	TYR	7.6
1	X	40	GLY	7.3
1	X	37	VAL	7.1
1	Y	109	GLY	6.3
1	X	27	LEU	6.1
1	X	86	ILE	5.7
1	X	11	ASP	5.7
1	X	52	VAL	5.4
1	X	91	PHE	5.3
1	X	19	GLU	5.1
1	X	25	GLU	5.1
1	X	75	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	X	20	ASN	5.1
1	X	87	ILE	4.9
1	X	55	GLN	4.9
1	X	204	GLN	4.9
1	X	10	PRO	4.8
1	X	74	VAL	4.8
1	X	33	ASN	4.7
1	X	12	GLN	4.6
1	X	59	GLU	4.6
1	X	34	ILE	4.6
1	X	3	GLU	4.6
1	X	18	SER	4.4
1	X	16	ALA	4.3
1	X	28	ASN	4.3
1	X	17	ILE	4.3
1	X	96	THR	4.2
1	X	29	LEU	4.2
1	X	21	THR	4.2
1	X	7	LEU	4.2
1	Y	607	THR	4.1
1	Y	606	GLY	4.1
1	X	84	ASP	4.0
1	X	46	LYS	4.0
1	X	70	ALA	3.9
1	Y	471	THR	3.9
1	X	47	CYS	3.9
1	X	80	TYR	3.9
1	X	53	ASP	3.9
1	Y	482	ASP	3.9
1	Y	625	HIS	3.9
1	X	30	ALA	3.9
1	X	22	ASN	3.8
1	Y	425	SER	3.7
1	Y	481	GLU	3.6
1	X	60	SER	3.5
1	Y	204	GLN	3.5
1	Y	467	LYS	3.5
1	Y	502	ILE	3.5
1	Y	622	THR	3.5
1	X	81	PRO	3.4
1	Y	426	GLU	3.4
1	X	5	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	157	ASN	3.3
1	X	6	VAL	3.3
1	X	83	SER	3.2
1	Y	277	PHE	3.2
1	Y	486	PHE	3.1
1	X	119	GLU	3.1
1	Y	245	ASP	3.1
1	X	139	ASP	3.0
1	X	76	ALA	3.0
1	Y	459	ALA	3.0
1	X	51	VAL	2.9
1	Y	117	ALA	2.9
1	Y	469	ASP	2.8
1	Y	529	ASP	2.7
1	X	63	LYS	2.7
1	X	92	ASP	2.7
1	X	138	LEU	2.7
1	Y	464	ARG	2.7
1	Y	119	GLU	2.6
1	X	104	ASP	2.6
1	X	93	SER	2.6
1	X	94	ARG	2.6
1	Y	148	LEU	2.5
1	Y	116	LEU	2.4
1	Y	209	LEU	2.4
1	X	630	VAL	2.4
1	Y	564	ILE	2.4
1	Y	624	LEU	2.3
1	Y	547	TYR	2.3
1	X	78	GLN	2.3
1	X	57	ARG	2.3
1	X	79	THR	2.3
1	Y	399	ALA	2.3
1	Y	480	GLY	2.3
1	Y	263	LYS	2.3
1	X	54	GLY	2.2
1	X	13	LYS	2.2
1	Y	628	PRO	2.2
1	Y	121	GLU	2.2
1	X	625	HIS	2.2
1	Y	605	VAL	2.2
1	Y	437	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	15	VAL	2.2
1	Y	430	LYS	2.2
1	Y	521	VAL	2.2
1	X	77	CYS	2.1
1	X	67	GLU	2.1
1	X	36	THR	2.1
1	X	148	LEU	2.1
1	X	9	LYS	2.1
1	Y	115	ASP	2.1
1	X	121	GLU	2.1
1	Y	610	MET	2.1
1	X	177	GLU	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
5	SO4	X	1632	5/5	0.71	0.40	8.90	68,75,105,114	0
5	SO4	X	1633	5/5	0.88	0.27	5.07	36,47,51,53	5
6	BU3	X	1638	6/6	0.79	0.21	4.74	59,66,72,74	0
5	SO4	X	1631	5/5	0.79	0.31	4.42	54,62,64,65	5
5	SO4	Y	1631	5/5	0.77	0.25	2.61	60,64,78,80	5
5	SO4	Y	1630	5/5	0.93	0.17	1.01	53,61,71,72	5
3	PO4	Y	801	5/5	0.94	0.12	-0.77	45,50,53,65	0
3	PO4	X	801	5/5	0.99	0.10	-1.45	32,36,40,42	0
2	FES	X	800	4/4	0.87	0.13	-1.63	120,122,125,134	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	X	1636	5/5	0.92	0.23	-	58,58,69,78	5
5	SO4	X	1635	5/5	0.94	0.23	-	37,39,56,56	5
5	SO4	X	1634	5/5	0.84	0.31	-	45,46,48,49	5
6	BU3	Y	1632	6/6	0.81	0.37	-	89,95,95,98	0
6	BU3	Y	1633	6/6	0.81	0.21	-	61,64,71,77	0
4	MG	X	802	1/1	0.96	0.05	-	34,34,34,34	0
4	MG	Y	802	1/1	0.94	0.04	-	53,53,53,53	0
5	SO4	X	1637	5/5	0.81	0.41	-	50,55,59,71	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.