



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:40 pm BST

PDB ID : 4D4P  
Title : Crystal Structure of the Kti11 Kti13 heterodimer Spacegroup P65  
Authors : Glatt, S.; Mueller, C.W.  
Deposited on : 2014-10-30  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

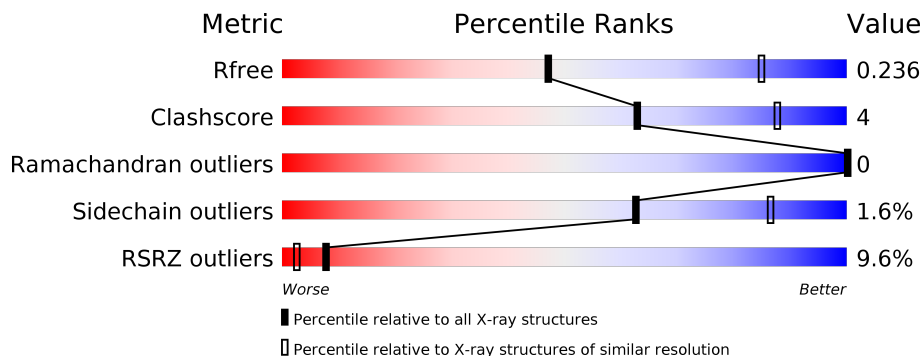
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. 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	427	
1	B	427	
1	C	427	
1	E	427	
1	G	427	
1	H	427	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12715 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 PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	Total 3178	C 1982	N 555	O 614	S 27	0	0	0
1	B	336	Total 2576	C 1603	N 471	O 484	S 18	0	0	0
1	C	76	Total 613	C 389	N 86	O 129	S 9	0	0	0
1	E	334	Total 2565	C 1597	N 469	O 481	S 18	0	0	0
1	G	409	Total 3152	C 1968	N 550	O 607	S 27	0	0	0
1	H	74	Total 602	C 382	N 84	O 127	S 9	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P31386
A	0	ALA	-	expression tag	UNP P31386
A	334	GLY	-	linker	UNP P31386
A	335	SER	-	linker	UNP P31386
A	336	GLY	-	linker	UNP P31386
A	337	SER	-	linker	UNP P31386
A	338	GLY	-	linker	UNP P31386
A	339	SER	-	linker	UNP P31386
A	340	GLY	-	linker	UNP P31386
A	341	SER	-	linker	UNP P31386
A	342	GLY	-	linker	UNP P31386
A	343	SER	-	linker	UNP P31386
B	-1	GLY	-	expression tag	UNP P31386
B	0	ALA	-	expression tag	UNP P31386
B	334	GLY	-	linker	UNP P31386
B	335	SER	-	linker	UNP P31386

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Chain	Residue	Modelled	Actual	Comment	Reference
B	336	GLY	-	linker	UNP P31386
B	337	SER	-	linker	UNP P31386
B	338	GLY	-	linker	UNP P31386
B	339	SER	-	linker	UNP P31386
B	340	GLY	-	linker	UNP P31386
B	341	SER	-	linker	UNP P31386
B	342	GLY	-	linker	UNP P31386
B	343	SER	-	linker	UNP P31386
C	-1	GLY	-	expression tag	UNP P31386
C	0	ALA	-	expression tag	UNP P31386
C	334	GLY	-	linker	UNP P31386
C	335	SER	-	linker	UNP P31386
C	336	GLY	-	linker	UNP P31386
C	337	SER	-	linker	UNP P31386
C	338	GLY	-	linker	UNP P31386
C	339	SER	-	linker	UNP P31386
C	340	GLY	-	linker	UNP P31386
C	341	SER	-	linker	UNP P31386
C	342	GLY	-	linker	UNP P31386
C	343	SER	-	linker	UNP P31386
E	-1	GLY	-	expression tag	UNP P31386
E	0	ALA	-	expression tag	UNP P31386
E	334	GLY	-	linker	UNP P31386
E	335	SER	-	linker	UNP P31386
E	336	GLY	-	linker	UNP P31386
E	337	SER	-	linker	UNP P31386
E	338	GLY	-	linker	UNP P31386
E	339	SER	-	linker	UNP P31386
E	340	GLY	-	linker	UNP P31386
E	341	SER	-	linker	UNP P31386
E	342	GLY	-	linker	UNP P31386
E	343	SER	-	linker	UNP P31386
G	-1	GLY	-	expression tag	UNP P31386
G	0	ALA	-	expression tag	UNP P31386
G	334	GLY	-	linker	UNP P31386
G	335	SER	-	linker	UNP P31386
G	336	GLY	-	linker	UNP P31386
G	337	SER	-	linker	UNP P31386
G	338	GLY	-	linker	UNP P31386
G	339	SER	-	linker	UNP P31386
G	340	GLY	-	linker	UNP P31386
G	341	SER	-	linker	UNP P31386

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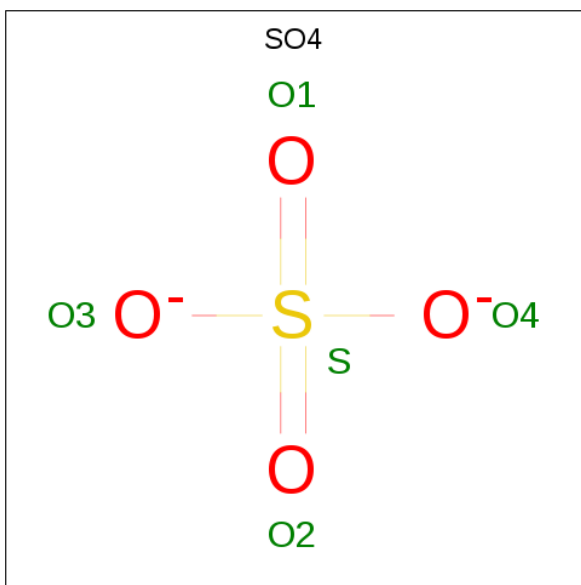
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Chain	Residue	Modelled	Actual	Comment	Reference
G	342	GLY	-	linker	UNP P31386
G	343	SER	-	linker	UNP P31386
H	-1	GLY	-	expression tag	UNP P31386
H	0	ALA	-	expression tag	UNP P31386
H	334	GLY	-	linker	UNP P31386
H	335	SER	-	linker	UNP P31386
H	336	GLY	-	linker	UNP P31386
H	337	SER	-	linker	UNP P31386
H	338	GLY	-	linker	UNP P31386
H	339	SER	-	linker	UNP P31386
H	340	GLY	-	linker	UNP P31386
H	341	SER	-	linker	UNP P31386
H	342	GLY	-	linker	UNP P31386
H	343	SER	-	linker	UNP P31386

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

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



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









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.06Å 152.06Å 203.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	110.61 – 3.00 131.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (110.61-3.00) 99.6 (131.69-3.00)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.208 , 0.234 0.210 , 0.236	Depositor DCC
$R_{free}$ test set	2660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.3	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: FE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/3253	0.39	1/4414 (0.0%)
1	B	0.20	0/2637	0.37	0/3580
1	C	0.21	0/629	0.38	0/853
1	E	0.21	0/2626	0.37	0/3565
1	G	0.23	0/3226	0.39	0/4376
1	H	0.26	0/616	0.40	0/833
All	All	0.22	0/12987	0.38	1/17621 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	CYS	C-N-CD	-8.07	102.85	120.60

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	3178	0	3004	28	0
1	B	2576	0	2471	24	0
1	C	613	0	547	4	0
1	E	2565	0	2461	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3152	0	2984	30	0
1	H	602	0	536	11	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	2	0
3	E	10	0	0	1	0
All	All	12715	0	12003	106	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 4.

All (106) 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:G:393:CYS:SG	1:G:395:LEU:HD23	2.00	1.00
1:E:296:GLU:OE1	1:G:394:SER:OG	1.99	0.81
1:G:224:VAL:HB	1:G:235:TRP:HB3	1.68	0.74
1:B:224:VAL:HB	1:B:235:TRP:HB3	1.68	0.74
1:G:395:LEU:N	1:G:395:LEU:HD22	2.03	0.73
1:A:224:VAL:HB	1:A:235:TRP:HB3	1.71	0.73
1:G:395:LEU:H	1:G:395:LEU:HD22	1.56	0.71
1:G:393:CYS:HB2	1:G:395:LEU:CD2	2.19	0.70
1:H:390:CYS:HB3	1:H:393:CYS:SG	2.32	0.69
1:H:393:CYS:SG	1:H:394:SER:N	2.68	0.66
1:A:189:LYS:NZ	1:C:348:ASP:OD2	2.30	0.64
1:A:294:TRP:HH2	1:C:370:CYS:HB3	1.61	0.63
1:A:296:GLU:HA	1:A:304:LYS:HB3	1.79	0.63
1:A:39:ARG:O	1:A:321:ARG:NH2	2.32	0.62
1:H:344:MET:HG3	1:H:387:VAL:HG21	1.81	0.62
1:E:107:ARG:NH1	3:E:1335:SO4:O3	2.33	0.61
1:E:224:VAL:HB	1:E:235:TRP:HB3	1.82	0.60
1:A:348:ASP:OD1	1:B:207:ARG:NH2	2.30	0.59
1:A:292:TRP:HB3	1:A:310:LEU:HD23	1.84	0.58
1:A:290:TYR:HB3	1:A:310:LEU:HB3	1.85	0.57
1:A:13:ARG:NH1	1:A:76:GLN:OE1	2.33	0.57
1:B:262:PRO:HG2	1:B:278:ALA:HB3	1.86	0.57
1:H:407:ALA:HA	1:H:410:TYR:HB2	1.86	0.57
1:A:107:ARG:NH1	3:A:1418:SO4:O1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:CYS:CB	1:G:395:LEU:HD23	2.36	0.56
1:G:395:LEU:CD2	1:G:395:LEU:H	2.19	0.55
1:B:107:ARG:NH1	3:B:1336:SO4:O4	2.40	0.55
1:B:92:VAL:HG23	1:B:101:ILE:HG22	1.88	0.55
1:H:386:LYS:HG2	1:H:401:PHE:HE1	1.73	0.54
1:G:292:TRP:HB3	1:G:310:LEU:HD23	1.89	0.53
1:G:296:GLU:HA	1:G:304:LYS:HB3	1.92	0.52
1:B:0:ALA:HB1	1:B:37:ILE:HD11	1.90	0.52
1:B:220:ARG:HE	1:B:223:LEU:HD11	1.75	0.51
1:G:395:LEU:N	1:G:395:LEU:CD2	2.73	0.51
1:B:57:LEU:HB3	1:B:83:VAL:HB	1.92	0.51
1:E:15:LEU:HB3	1:E:17:LEU:HG	1.93	0.51
1:B:125:LEU:HD13	1:B:132:ILE:HD13	1.92	0.51
1:G:335:SER:OG	1:G:336:GLY:N	2.44	0.51
1:B:279:ASN:ND2	1:G:249:THR:O	2.42	0.51
1:E:12:GLN:OE1	1:E:76:GLN:NE2	2.43	0.51
1:C:345:SER:HB3	1:E:315:GLN:HB3	1.93	0.50
1:A:322:VAL:HG12	1:A:331:ILE:HG12	1.94	0.50
1:B:15:LEU:HB3	1:B:17:LEU:HG	1.93	0.50
1:G:294:TRP:HH2	1:H:370:CYS:HB3	1.76	0.49
1:B:215:LYS:H	1:B:215:LYS:HD2	1.76	0.49
1:A:191:PHE:HA	1:A:206:GLY:HA3	1.95	0.49
1:A:249:THR:O	1:E:315:GLN:NE2	2.32	0.49
1:B:323:PHE:HB2	1:B:330:TRP:HB2	1.95	0.49
1:G:390:CYS:SG	1:G:393:CYS:SG	3.11	0.49
1:A:57:LEU:HG	1:A:89:VAL:HG21	1.94	0.48
1:G:15:LEU:HB3	1:G:17:LEU:HG	1.95	0.48
1:A:147:THR:HG23	1:A:177:THR:HB	1.95	0.48
1:E:102:VAL:HG22	1:E:108:VAL:HG22	1.95	0.47
1:G:374:PHE:HE1	1:G:395:LEU:HB3	1.79	0.47
1:A:323:PHE:HB2	1:A:330:TRP:HB2	1.97	0.47
1:G:132:ILE:HG12	1:G:145:GLN:HG3	1.95	0.47
1:G:374:PHE:CE1	1:G:395:LEU:HB3	2.50	0.46
1:G:43:CYS:HG	1:G:330:TRP:HE1	1.62	0.46
1:E:296:GLU:HA	1:E:304:LYS:HB3	1.97	0.46
1:A:16:GLY:HA3	1:A:80:TRP:NE1	2.32	0.45
1:A:381:MET:HB2	1:A:381:MET:HE3	1.70	0.45
1:A:194:ILE:HD12	1:A:203:HIS:HB3	1.99	0.44
1:E:247:ARG:NH2	1:G:346:THR:O	2.50	0.44
1:A:41:ILE:HG12	1:A:50:MET:HG2	1.99	0.44
1:H:390:CYS:HA	1:H:391:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MET:HB2	1:A:58:VAL:HG13	2.00	0.44
1:B:238:ARG:NH1	3:B:1337:SO4:O3	2.51	0.44
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.84	0.43
1:B:333:LEU:HD13	1:H:343:SER:HB3	1.99	0.43
1:B:24:ASP:HB3	1:B:304:LYS:HE2	2.00	0.43
1:B:64:ARG:HG2	1:B:75:ARG:HD2	1.99	0.43
1:C:376:ILE:HG21	1:C:399:VAL:HG21	2.01	0.43
1:G:146:GLY:O	1:G:148:ARG:N	2.47	0.43
1:E:274:ILE:HD13	1:E:329:THR:HG23	1.99	0.43
1:A:357:PHE:HZ	1:A:413:ALA:HB2	1.84	0.43
1:H:376:ILE:HG21	1:H:399:VAL:HG21	1.99	0.42
1:E:204:ALA:HB3	1:E:214:LEU:HD22	2.01	0.42
1:G:242:VAL:HB	1:G:254:PHE:CG	2.55	0.42
1:G:274:ILE:HD13	1:G:329:THR:HG23	2.01	0.42
1:B:44:GLY:HA3	1:B:47:HIS:CE1	2.54	0.42
1:H:372:ASP:OD1	1:H:373:ARG:N	2.45	0.42
1:B:1:MET:HG3	1:B:35:GLY:HA2	2.01	0.42
1:E:191:PHE:HA	1:E:206:GLY:HA3	2.02	0.42
1:A:272:HIS:CG	1:A:299:ASN:HD22	2.38	0.41
1:B:296:GLU:HA	1:B:304:LYS:HB3	2.01	0.41
1:E:170:GLU:HA	1:E:171:PRO:HD3	1.88	0.41
1:A:101:ILE:HG12	1:A:109:TRP:HB2	2.02	0.41
1:E:234:LEU:HB2	1:E:243:GLU:HB2	2.01	0.41
1:E:294:TRP:CZ2	1:G:395:LEU:HD21	2.55	0.41
1:G:177:THR:HB	1:G:179:SER:H	1.84	0.41
1:G:162:GLU:HA	1:G:163:PRO:HA	1.74	0.41
1:A:3:CYS:HB2	1:A:333:LEU:HB2	2.03	0.41
1:B:29:SER:OG	1:B:80:TRP:NE1	2.45	0.41
1:G:290:TYR:HB3	1:G:310:LEU:HB3	2.02	0.41
1:E:177:THR:N	1:E:178:GLY:HA2	2.36	0.41
1:B:241:THR:OG1	1:B:242:VAL:N	2.53	0.41
1:A:170:GLU:HA	1:A:171:PRO:HD3	1.93	0.41
1:E:97:ASP:O	1:E:113:GLY:N	2.54	0.41
1:A:392:SER:C	1:A:393:CYS:SG	2.99	0.41
1:A:12:GLN:OE1	1:A:76:GLN:NE2	2.54	0.41
1:E:242:VAL:HB	1:E:254:PHE:CG	2.56	0.41
1:G:366:TYR:HA	1:G:367:PRO:HD3	1.98	0.41
1:H:380:ASP:HB3	1:H:385:GLU:OE1	2.21	0.41
1:E:128:ASN:N	1:E:128:ASN:OD1	2.54	0.40
1:E:294:TRP:HH2	1:G:370:CYS:HB3	1.86	0.40
1:B:204:ALA:HB3	1:B:214:LEU:HD22	2.02	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	409/427 (96%)	384 (94%)	25 (6%)	0	100	100
1	B	334/427 (78%)	312 (93%)	22 (7%)	0	100	100
1	C	74/427 (17%)	72 (97%)	2 (3%)	0	100	100
1	E	332/427 (78%)	309 (93%)	23 (7%)	0	100	100
1	G	403/427 (94%)	367 (91%)	36 (9%)	0	100	100
1	H	70/427 (16%)	61 (87%)	9 (13%)	0	100	100
All	All	1622/2562 (63%)	1505 (93%)	117 (7%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/351 (98%)	340 (99%)	3 (1%)	78	92
1	B	275/351 (78%)	272 (99%)	3 (1%)	73	90
1	C	70/351 (20%)	69 (99%)	1 (1%)	67	88
1	E	274/351 (78%)	272 (99%)	2 (1%)	84	94
1	G	341/351 (97%)	334 (98%)	7 (2%)	53	82
1	H	69/351 (20%)	63 (91%)	6 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1372/2106 (65%)	1350 (98%)	22 (2%)	62 86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	SER
1	A	394	SER
1	A	396	MET
1	B	78	HIS
1	B	118	PHE
1	B	281	GLU
1	C	361	ASN
1	E	28	ARG
1	E	52	THR
1	G	166	ARG
1	G	257	GLU
1	G	321	ARG
1	G	349	GLU
1	G	392	SER
1	G	393	CYS
1	G	394	SER
1	H	357	PHE
1	H	380	ASP
1	H	401	PHE
1	H	406	LEU
1	H	410	TYR
1	H	412	GLU

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

Mol	Chain	Res	Type
1	B	27	GLN
1	B	221	HIS

### 5.3.3 RNA ⓘ

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	SO4	E	1336	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	E	1335	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	1337	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	1418	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	1336	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1335	SO4	1	0
3	B	1337	SO4	1	0
3	A	1418	SO4	1	0
3	B	1336	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	413/427 (96%)	0.77	32 (7%) 13 4	60, 97, 139, 214	0
1	B	336/427 (78%)	0.87	21 (6%) 20 6	65, 88, 129, 169	0
1	C	76/427 (17%)	0.83	3 (3%) 39 15	72, 85, 115, 135	0
1	E	334/427 (78%)	0.92	33 (9%) 7 2	66, 98, 147, 241	0
1	G	409/427 (95%)	0.93	57 (13%) 2 1	70, 113, 161, 239	0
1	H	74/427 (17%)	0.92	12 (16%) 1 0	77, 140, 189, 210	0
All	All	1642/2562 (64%)	0.87	158 (9%) 8 2	60, 99, 154, 241	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	160	LEU	7.4
1	E	129	ASP	5.6
1	G	37	ILE	5.1
1	G	33	ASP	4.8
1	E	125	LEU	4.4
1	G	99	THR	4.4
1	G	132	ILE	4.0
1	G	191	PHE	4.0
1	H	378	LEU	4.0
1	G	32	GLY	3.9
1	G	100	VAL	3.8
1	A	129	ASP	3.7
1	A	115	CYS	3.7
1	B	201	ILE	3.6
1	G	150	TYR	3.6
1	G	212	PHE	3.6
1	E	68	LEU	3.5
1	G	344	MET	3.5
1	E	78	HIS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	409	TYR	3.4
1	G	173	LEU	3.4
1	G	68	LEU	3.3
1	H	366	TYR	3.3
1	E	109	TRP	3.3
1	E	48	SER	3.1
1	E	148	ARG	3.1
1	H	364	PHE	3.1
1	G	193	VAL	3.1
1	G	47	HIS	3.0
1	C	389	VAL	3.0
1	B	331	ILE	2.9
1	G	85	VAL	2.9
1	G	168	LEU	2.9
1	G	129	ASP	2.9
1	B	49	VAL	2.9
1	H	400	VAL	2.8
1	B	166	ARG	2.8
1	E	294	TRP	2.8
1	H	389	VAL	2.8
1	A	150	TYR	2.8
1	G	58	VAL	2.8
1	G	263	ILE	2.8
1	G	399	VAL	2.8
1	A	132	ILE	2.7
1	B	330	TRP	2.7
1	E	160	LEU	2.7
1	G	118	PHE	2.7
1	G	401	PHE	2.7
1	B	263	ILE	2.7
1	G	140	ASN	2.7
1	G	7	PHE	2.6
1	G	291	CYS	2.6
1	E	132	ILE	2.6
1	A	89	VAL	2.6
1	E	117	GLU	2.6
1	G	67	GLU	2.6
1	A	116	TYR	2.6
1	B	83	VAL	2.6
1	E	150	TYR	2.6
1	G	133	ALA	2.6
1	H	401	PHE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	144	VAL	2.6
1	G	1	MET	2.5
1	G	378	LEU	2.5
1	A	92	VAL	2.5
1	A	114	GLY	2.5
1	A	352	ILE	2.5
1	B	132	ILE	2.5
1	A	144	VAL	2.5
1	G	329	THR	2.5
1	E	292	TRP	2.5
1	G	151	GLY	2.5
1	A	163	PRO	2.5
1	E	161	GLN	2.5
1	A	415	ILE	2.5
1	A	229	TRP	2.4
1	B	321	ARG	2.4
1	E	232	ILE	2.4
1	E	245	PHE	2.4
1	B	291	CYS	2.4
1	A	261	PHE	2.4
1	A	113	GLY	2.4
1	G	182	VAL	2.4
1	G	216	GLN	2.4
1	G	364	PHE	2.4
1	A	182	VAL	2.4
1	H	367	PRO	2.4
1	G	49	VAL	2.4
1	B	194	ILE	2.4
1	A	90	VAL	2.3
1	G	145	GLN	2.3
1	G	330	TRP	2.3
1	E	201	ILE	2.3
1	G	232	ILE	2.3
1	A	409	TYR	2.3
1	G	409	TYR	2.3
1	H	393	CYS	2.3
1	G	223	LEU	2.3
1	G	299	ASN	2.3
1	G	235	TRP	2.3
1	H	397	ILE	2.3
1	A	142	VAL	2.3
1	A	263	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	399	VAL	2.3
1	B	109	TRP	2.3
1	G	292	TRP	2.3
1	E	42	ALA	2.3
1	A	364	PHE	2.3
1	B	9	SER	2.2
1	E	310	LEU	2.2
1	B	160	LEU	2.2
1	B	254	PHE	2.2
1	E	261	PHE	2.2
1	G	347	TYR	2.2
1	B	129	ASP	2.2
1	G	101	ILE	2.2
1	A	223	LEU	2.2
1	E	331	ILE	2.2
1	G	42	ALA	2.2
1	E	26	PRO	2.2
1	G	161	GLN	2.2
1	G	144	VAL	2.2
1	A	378	LEU	2.2
1	C	388	ALA	2.2
1	G	245	PHE	2.2
1	A	248	GLY	2.1
1	E	133	ALA	2.1
1	G	93	ALA	2.1
1	E	289	VAL	2.1
1	A	17	LEU	2.1
1	E	33	ASP	2.1
1	A	294	TRP	2.1
1	B	327	ALA	2.1
1	E	40	LYS	2.1
1	G	80	TRP	2.1
1	A	195	VAL	2.1
1	A	273	GLY	2.1
1	G	73	ALA	2.1
1	B	294	TRP	2.1
1	H	357	PHE	2.1
1	E	327	ALA	2.1
1	E	269	GLY	2.1
1	A	9	SER	2.1
1	B	77	VAL	2.1
1	B	253	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	313	VAL	2.1
1	G	386	LYS	2.1
1	G	360	GLU	2.0
1	G	272	HIS	2.0
1	G	189	LYS	2.0
1	E	242	VAL	2.0
1	C	364	PHE	2.0
1	A	122	HIS	2.0
1	A	297	HIS	2.0
1	E	166	ARG	2.0
1	A	201	ILE	2.0
1	E	4	VAL	2.0
1	E	49	VAL	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1418	5/5	0.82	0.20	156,156,156,156	0
3	SO4	E	1335	5/5	0.89	0.14	163,163,163,163	0
3	SO4	B	1336	5/5	0.90	0.19	135,135,135,135	0
2	FE	H	501	1/1	0.91	0.21	102,102,102,102	0
2	FE	A	501	1/1	0.93	0.18	109,109,109,109	0
3	SO4	B	1337	5/5	0.94	0.24	117,117,117,117	0
3	SO4	E	1336	5/5	0.94	0.15	121,121,121,121	0
2	FE	G	501	1/1	0.97	0.17	133,133,133,133	0
2	FE	C	501	1/1	1.00	0.19	87,87,87,87	0

## 6.5 Other polymers

There are no such residues in this entry.