



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:46 AM UTC

PDB ID : 4D4P / pdb_00004d4p
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

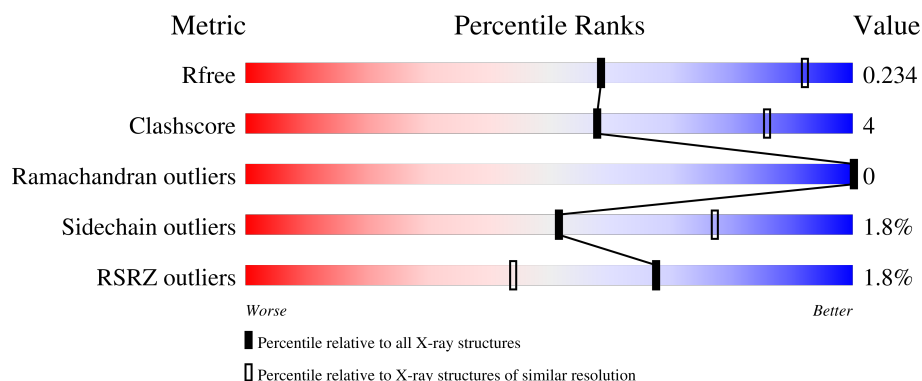
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	84% 12% .
1	B	427	68% 11% 21%
1	C	427	15% . 82%
1	E	427	70% 8% 22%
1	G	427	86% 10% .

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Mol	Chain	Length	Quality of chain
1	H	427	2%12%5%83%

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

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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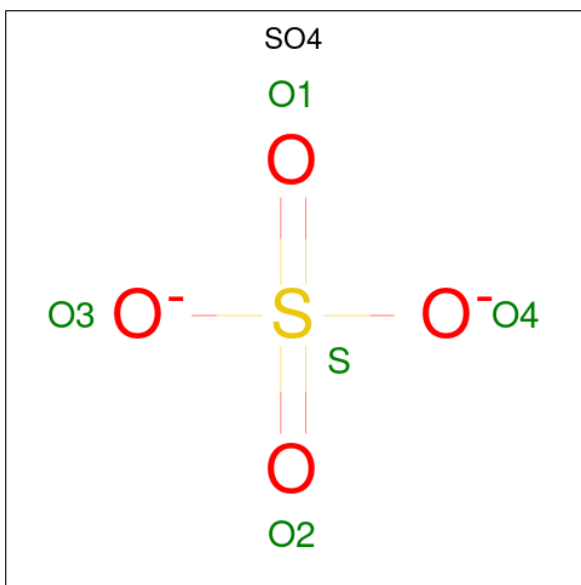
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Chain	Residue	Modelled	Actual	Comment	Reference
G	342	GLY	-	linker	UNP P31386
G	343	SER	-	linker	UNP P31386
H	-1	GLY	-	expression tag	UNP P31386
H	0	ALA	-	expression tag	UNP P31386
H	334	GLY	-	linker	UNP P31386
H	335	SER	-	linker	UNP P31386
H	336	GLY	-	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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

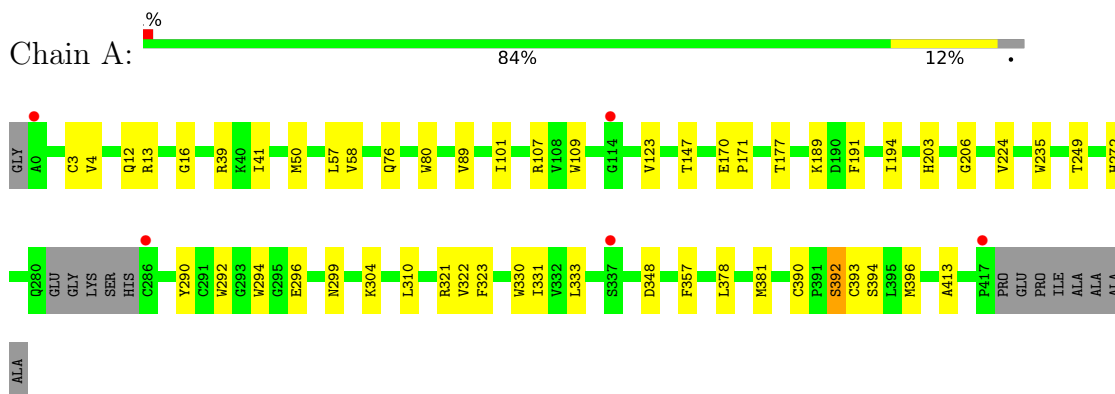


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

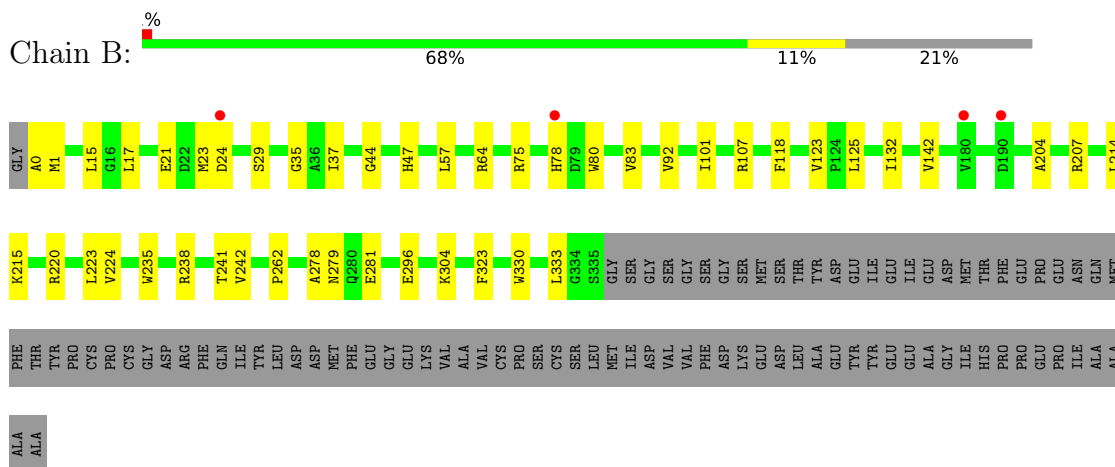
3 Residue-property plots

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

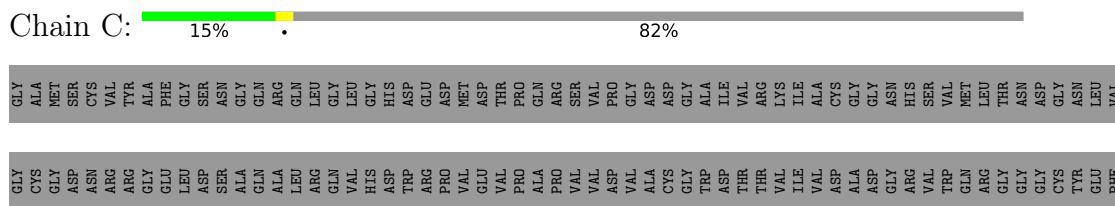
- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3



- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3

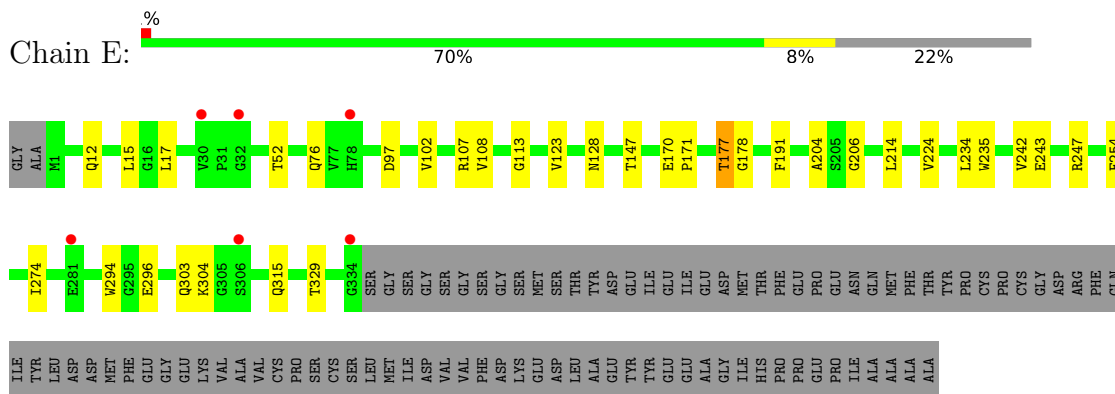


- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3

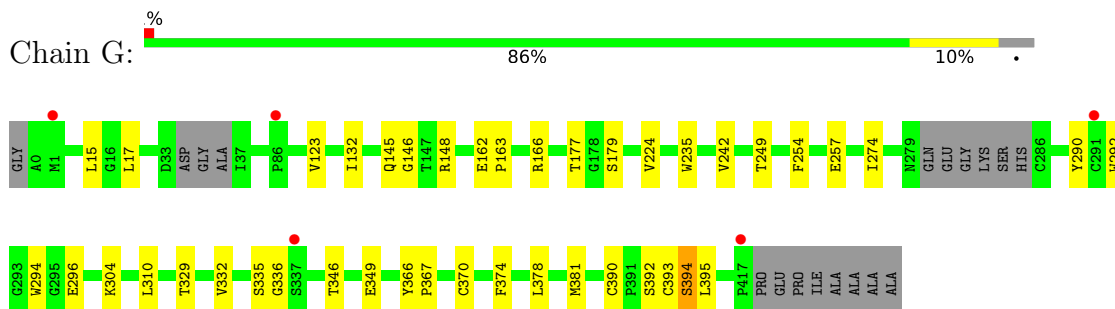




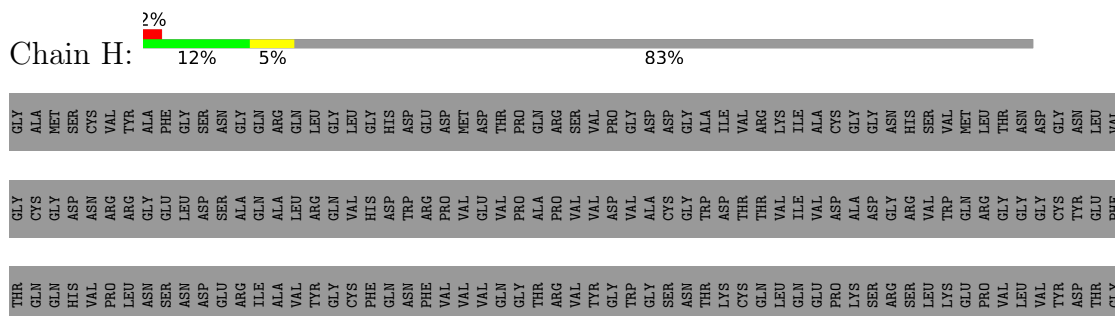
- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3



- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3



- Molecule 1: PROTEIN ATS1, DIPHTHAMIDE BIOSYNTHESIS PROTEIN 3



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	152.06Å 152.06Å 203.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	110.61 – 3.00 110.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (110.61-3.00) 99.6 (110.61-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.234 0.211 , 0.234	Depositor DCC
R_{free} test set	2660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12715	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FE

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	0.29	0/3253	0.69	1/4414 (0.0%)
1	B	0.24	0/2637	0.68	0/3580
1	C	0.27	0/629	0.79	2/853 (0.2%)
1	E	0.26	0/2626	0.67	1/3565 (0.0%)
1	G	0.29	0/3226	0.70	0/4376
1	H	0.34	0/616	0.81	2/833 (0.2%)
All	All	0.28	0/12987	0.70	6/17621 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	HIS	CA-C-N	5.97	124.02	119.66
1	C	416	HIS	C-N-CA	5.97	124.02	119.66
1	H	358	GLU	CA-C-N	5.92	126.07	119.32
1	H	358	GLU	C-N-CA	5.92	126.07	119.32
1	A	390	CYS	C-N-CD	-5.40	102.85	125.00
1	E	177	THR	N-CA-C	5.35	116.80	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3178	0	3004	29	0
1	B	2576	0	2471	25	0
1	C	613	0	547	5	0
1	E	2565	0	2461	21	0
1	G	3152	0	2984	30	0
1	H	602	0	536	12	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	110	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 (110) 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:HD22	1:G:395:LEU:N	2.03	0.73
1:A:224:VAL:HB	1:A:235:TRP:HB3	1.71	0.73
1:G:395:LEU:HD22	1:G:395:LEU:H	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:A:378:LEU:HA	1:A:381:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:393:CYS:CB	1:G:395:LEU:HD23	2.36	0.56
1:G:395:LEU:H	1:G:395:LEU:CD2	2.19	0.55
1:B:107:ARG:NH1	3:B:1336:SO4:O4	2.40	0.55
1:H:378:LEU:HA	1:H:381:MET:HE3	1.88	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:G:378:LEU:HA	1:G:381:MET:HE2	1.92	0.49
1:G:390:CYS:SG	1:G:393:CYS:SG	3.11	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: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:A:4:VAL:HG11	1:A:50:MET:HE1	1.97	0.46
1:G:374:PHE:CE1	1:G:395:LEU:HB3	2.50	0.46
1:C:372:ASP:OD2	1:C:392:SER:OG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:GLU:HA	1:E:304:LYS:HB3	1.97	0.46
1:A:392:SER:C	1:A:393:CYS:SG	2.99	0.45
1:A:16:GLY:HA3	1:A:80:TRP:NE1	2.32	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
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:21:GLU:HB3	1:B:23:MET:HE3	2.00	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:12:GLN:OE1	1:A:76:GLN:NE2	2.54	0.41
1:A:170:GLU:HA	1:A:171:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:ASP:O	1:E:113:GLY:N	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: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
1:E:128:ASN:OD1	1:E:128:ASN:N	2.54	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%)	339 (99%)	4 (1%)	63	82
1	B	275/351 (78%)	270 (98%)	5 (2%)	51	77
1	C	70/351 (20%)	68 (97%)	2 (3%)	37	70
1	E	274/351 (78%)	270 (98%)	4 (2%)	57	80
1	G	341/351 (97%)	334 (98%)	7 (2%)	47	75
1	H	69/351 (20%)	66 (96%)	3 (4%)	26	60
All	All	1372/2106 (65%)	1347 (98%)	25 (2%)	51	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	392	SER
1	A	394	SER
1	A	396	MET
1	B	78	HIS
1	B	118	PHE
1	B	123	VAL
1	B	142	VAL
1	B	281	GLU
1	C	361	ASN
1	C	404	GLU
1	E	52	THR
1	E	123	VAL
1	E	147	THR
1	E	303	GLN
1	G	123	VAL
1	G	166	ARG
1	G	257	GLU
1	G	332	VAL
1	G	349	GLU
1	G	392	SER
1	G	394	SER
1	H	406	LEU
1	H	410	TYR
1	H	412	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	122	HIS
1	A	311	GLN
1	B	27	GLN
1	B	121	GLN
1	E	27	GLN
1	E	122	HIS
1	E	203	HIS
1	G	46	ASN
1	G	56	ASN
1	G	315	GLN
1	H	361	ASN
1	H	362	GLN

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 oligosaccharides 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	0.24	0	6,6,6	0.07	0
3	SO4	A	1418	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	1336	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	E	1335	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	1337	-	4,4,4	0.24	0	6,6,6	0.07	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	A	1418	SO4	1	0
3	B	1336	SO4	1	0
3	E	1335	SO4	1	0
3	B	1337	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, 95th 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 ²)	Q<0.9
1	A	413/427 (96%)	0.13	5 (1%) 76 55	60, 97, 139, 214	0
1	B	336/427 (78%)	0.06	4 (1%) 76 55	65, 88, 129, 169	0
1	C	76/427 (17%)	-0.21	1 (1%) 75 53	72, 85, 115, 135	0
1	E	334/427 (78%)	0.10	6 (1%) 67 44	66, 98, 147, 241	0
1	G	409/427 (95%)	0.24	5 (1%) 76 55	70, 113, 161, 239	0
1	H	74/427 (17%)	0.82	9 (12%) 8 5	77, 140, 189, 210	0
All	All	1642/2562 (64%)	0.15	30 (1%) 67 44	60, 99, 154, 241	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	GLY	4.3
1	H	417	PRO	4.0
1	H	393	CYS	3.9
1	E	78	HIS	3.8
1	G	1	MET	3.6
1	H	343	SER	3.4
1	H	406	LEU	3.2
1	H	415	ILE	3.1
1	B	78	HIS	3.1
1	A	114	GLY	3.0
1	C	343	SER	2.9
1	G	86	PRO	2.9
1	A	286	CYS	2.8
1	A	0	ALA	2.7
1	G	417	PRO	2.7
1	E	32	GLY	2.6
1	B	24	ASP	2.6
1	A	417	PRO	2.6
1	H	378	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	337	SER	2.5
1	H	385	GLU	2.5
1	E	306	SER	2.4
1	G	291	CYS	2.3
1	H	400	VAL	2.3
1	B	190	ASP	2.2
1	H	409	TYR	2.2
1	E	281	GLU	2.2
1	G	337	SER	2.0
1	B	180	VAL	2.0
1	E	30	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
3	SO4	A	1418	5/5	0.75	0.08	156,156,156,156	0
3	SO4	E	1335	5/5	0.76	0.07	163,163,163,163	0
3	SO4	B	1336	5/5	0.82	0.06	135,135,135,135	0
3	SO4	B	1337	5/5	0.91	0.12	117,117,117,117	0
3	SO4	E	1336	5/5	0.94	0.08	121,121,121,121	0
2	FE	H	501	1/1	0.95	0.08	102,102,102,102	0
2	FE	A	501	1/1	0.97	0.07	109,109,109,109	0
2	FE	G	501	1/1	0.99	0.07	133,133,133,133	0
2	FE	C	501	1/1	1.00	0.07	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.