



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:58 PM GMT

PDB ID : 2Y0F
Title : STRUCTURE OF GCPE (ISPG) FROM THERMUS THERMOPHILUS HB27
Authors : Rekittke, I.; Nonaka, T.; Wiesner, J.; Demmer, U.; Warkentin, E.; Jomaa, H.; Ermler, U.
Deposited on : 2010-12-02
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

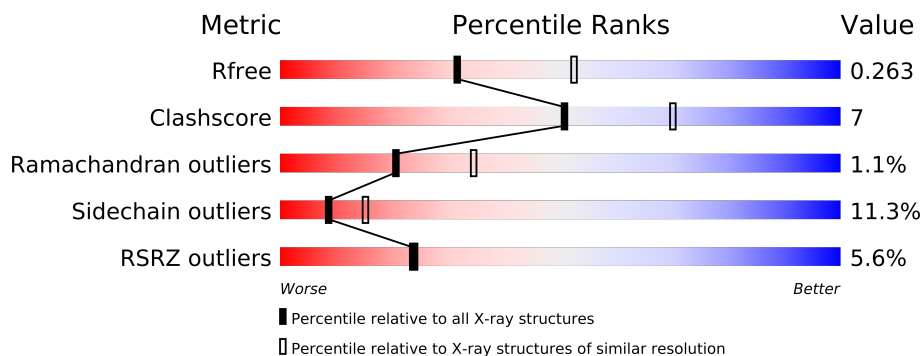
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SF4	D	501	-	X

2 Entry composition i

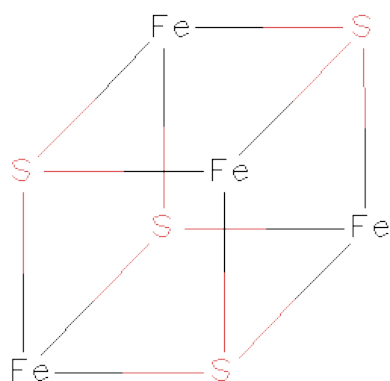
There are 3 unique types of molecules in this entry. The entry contains 12245 atoms, of which 0 are hydrogen and 0 are deuterium.

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 4-HYDROXY-3-METHYLBUT-2-EN-1-YLDIPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3077	1942	556	567	12			
1	B	394	Total	C	N	O	S	0	0	0
			3005	1900	538	555	12			
1	C	392	Total	C	N	O	S	0	0	0
			2995	1896	536	551	12			
1	D	393	Total	C	N	O	S	0	0	0
			3001	1898	537	554	12			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is water.

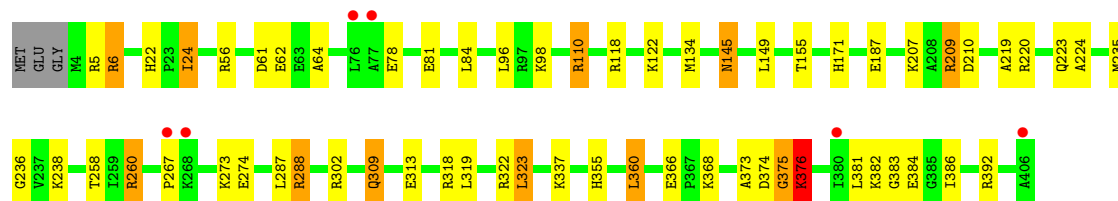
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	35	Total	O	0	0
			35	35		
3	C	28	Total	O	0	0
			28	28		
3	D	16	Total	O	0	0
			16	16		

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.

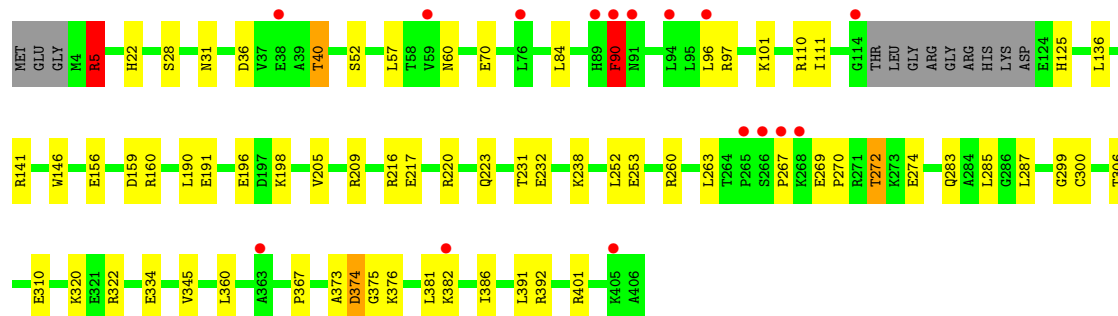
• Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YLDIPHOSPHATE SYNTHASE

Chain A: 



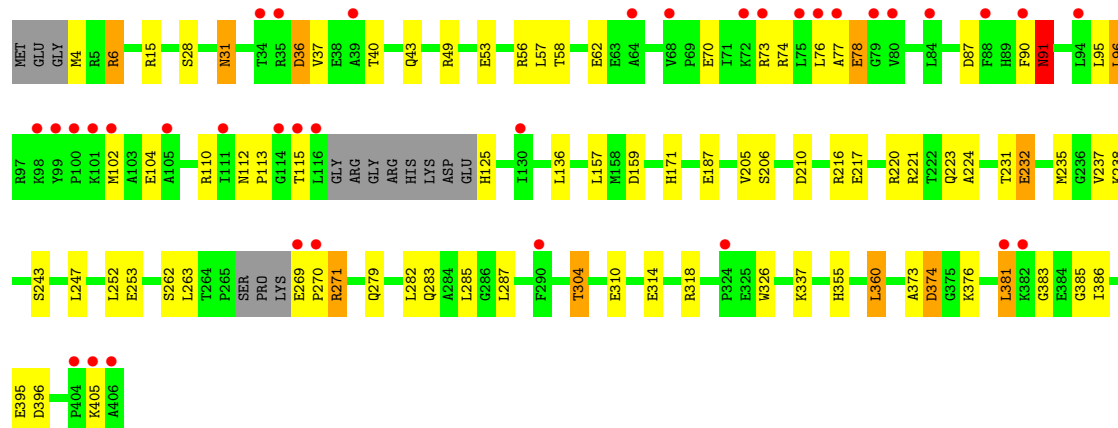
• Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YLDIPHOSPHATE SYNTHASE

Chain B: 



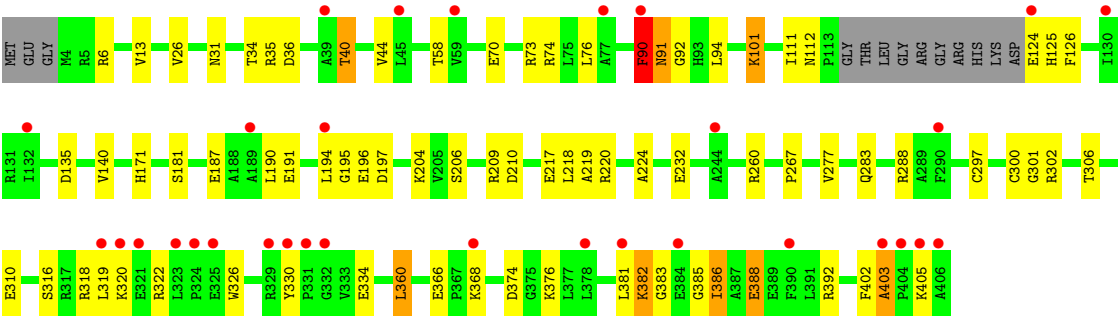
• Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YLDIPHOSPHATE SYNTHASE

Chain C: 



● Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YLDIPHOSPHATE SYNTHASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.50Å 130.97Å 101.26Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 48.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.50) 96.1 (48.20-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.199 , 0.263 0.199 , 0.263	Depositor DCC
R_{free} test set	3609 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 71545 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12245	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.86	2/3134 (0.1%)	0.95	11/4245 (0.3%)
1	B	0.79	2/3060 (0.1%)	0.89	6/4146 (0.1%)
1	C	1.04	15/3049 (0.5%)	0.92	7/4130 (0.2%)
1	D	0.70	1/3056 (0.0%)	0.81	2/4141 (0.0%)
All	All	0.86	20/12299 (0.2%)	0.90	26/16662 (0.2%)

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	A	0	1
1	C	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CD-OE1	14.95	1.42	1.25
1	C	70	GLU	CD-OE1	14.71	1.41	1.25
1	C	70	GLU	CD-OE2	12.50	1.39	1.25
1	C	78	GLU	C-N	11.64	1.53	1.33
1	C	77	ALA	C-O	11.23	1.44	1.23
1	C	77	ALA	C-N	11.13	1.59	1.34
1	A	375	GLY	N-CA	9.15	1.59	1.46
1	C	37	VAL	CB-CG2	-8.05	1.35	1.52
1	C	62	GLU	CG-CD	7.97	1.64	1.51
1	C	78	GLU	CG-CD	7.47	1.63	1.51
1	C	37	VAL	CB-CG1	7.36	1.68	1.52
1	C	37	VAL	CA-CB	7.18	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	CYS	CB-SG	-6.37	1.71	1.82
1	C	36	ASP	C-O	6.29	1.35	1.23
1	B	146	TRP	CB-CG	5.92	1.60	1.50
1	C	62	GLU	CD-OE1	5.85	1.32	1.25
1	C	31	ASN	CB-CG	5.61	1.64	1.51
1	B	70	GLU	CG-CD	5.53	1.60	1.51
1	A	375	GLY	CA-C	5.18	1.60	1.51
1	C	49	ARG	CZ-NH1	5.13	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	6	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	6	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	C	6	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	D	360	LEU	CA-CB-CG	-7.83	97.29	115.30
1	B	360	LEU	CA-CB-CG	-7.27	98.57	115.30
1	B	141	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	381	LEU	CA-CB-CG	6.77	130.88	115.30
1	C	360	LEU	CA-CB-CG	-6.33	100.74	115.30
1	A	376	LYS	N-CA-C	6.22	127.80	111.00
1	A	209	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	360	LEU	CA-CB-CG	-6.10	101.28	115.30
1	C	96	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	322	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	110	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	267	PRO	N-CA-CB	5.98	110.48	103.30
1	B	267	PRO	N-CA-CB	5.88	110.36	103.30
1	A	267	PRO	N-CA-CB	5.59	110.01	103.30
1	B	5	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	209	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	110	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	77	ALA	O-C-N	5.40	131.33	122.70
1	A	134	MET	CG-SD-CE	5.39	108.83	100.20
1	C	221	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	323	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	141	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ASP	Peptide
1	C	304	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3077	0	0	30	0
1	B	3005	0	0	17	0
1	C	2995	0	0	31	0
1	D	3001	0	0	20	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	56	0	0	4	0
3	B	35	0	0	2	0
3	C	28	0	0	7	0
3	D	16	0	0	2	0
All	All	12245	0	0	90	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:381:LEU:O	1:D:383:GLY:N	1.97	0.96
1:C:223:GLN:NE2	3:C:2019:HOH:O	2.03	0.90
1:A:56:ARG:NH2	3:A:2009:HOH:O	2.18	0.76
1:C:374:ASP:OD2	3:C:2028:HOH:O	2.06	0.74
1:D:6:ARG:NH1	1:D:219:ALA:O	2.21	0.73
1:D:36:ASP:O	1:D:40:THR:CG2	2.37	0.72
1:C:6:ARG:NH2	1:C:224:ALA:O	2.24	0.70
1:A:302:ARG:NH1	1:B:159:ASP:OD1	2.25	0.70
1:A:219:ALA:O	3:C:2019:HOH:O	2.12	0.68
1:A:145:ASN:ND2	3:A:2026:HOH:O	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:5:ARG:NH2	1:B:22:HIS:O	2.31	0.64
1:D:195:GLY:C	1:D:197:ASP:N	2.50	0.64
1:C:159:ASP:OD1	1:D:302:ARG:NH1	2.31	0.63
1:A:235:MET:CG	1:A:236:GLY:N	2.63	0.62
1:C:223:GLN:NE2	3:C:2018:HOH:O	2.34	0.61
1:A:209:ARG:NH1	1:B:285:LEU:O	2.33	0.61
1:B:216:ARG:NH2	1:B:253:GLU:OE2	2.33	0.61
1:A:381:LEU:O	1:A:383:GLY:N	2.33	0.61
1:B:90:PHE:CD1	1:B:90:PHE:N	2.68	0.60
1:B:36:ASP:O	1:B:40:THR:CG2	2.50	0.59
1:D:91:ASN:CB	3:D:2005:HOH:O	2.50	0.59
1:C:271:ARG:CG	1:C:271:ARG:NH1	2.67	0.57
1:C:217:GLU:OE2	1:C:220:ARG:NH1	2.38	0.57
1:B:31:ASN:ND2	1:B:269:GLU:O	2.39	0.56
1:C:374:ASP:N	1:C:374:ASP:OD1	2.38	0.56
1:A:373:ALA:N	1:A:375:GLY:O	2.39	0.56
1:A:5:ARG:NH1	1:A:22:HIS:O	2.39	0.55
1:C:91:ASN:C	1:C:91:ASN:ND2	2.59	0.55
1:A:6:ARG:NH2	1:A:224:ALA:O	2.40	0.55
1:A:171:HIS:NE2	1:A:210:ASP:OD2	2.39	0.55
1:C:110:ARG:NH2	1:C:112:ASN:OD1	2.40	0.55
1:A:223:GLN:NE2	3:C:2018:HOH:O	2.41	0.54
1:C:90:PHE:O	1:C:91:ASN:CB	2.56	0.54
1:C:381:LEU:O	1:C:383:GLY:N	2.40	0.54
1:A:337:LYS:N	1:A:355:HIS:CD2	2.76	0.54
1:C:205:VAL:CG1	1:C:206:SER:N	2.71	0.53
1:D:326:TRP:O	1:D:330:TYR:N	2.42	0.53
1:A:220:ARG:NH1	1:C:187:GLU:OE2	2.42	0.52
1:A:207:LYS:NZ	3:A:2043:HOH:O	2.42	0.52
1:B:283:GLN:NE2	3:B:2026:HOH:O	2.42	0.52
1:A:238:LYS:NZ	3:A:2050:HOH:O	2.42	0.52
1:D:402:PHE:O	1:D:403:ALA:CB	2.57	0.52
1:D:6:ARG:NH2	1:D:224:ALA:O	2.44	0.51
1:C:337:LYS:N	1:C:355:HIS:CD2	2.79	0.50
1:D:366:GLU:O	1:D:368:LYS:N	2.44	0.50
1:A:309:GLN:NE2	1:A:309:GLN:CA	2.75	0.50
1:A:260:ARG:NH2	1:A:274:GLU:OE1	2.45	0.50
1:C:74:ARG:O	1:C:78:GLU:N	2.45	0.50
1:A:288:ARG:CG	1:A:288:ARG:NH1	2.75	0.49
1:C:205:VAL:CG1	1:C:210:ASP:CB	2.91	0.49
1:B:260:ARG:NH2	1:B:274:GLU:OE2	2.45	0.49
1:C:216:ARG:NH2	1:C:253:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:376:LYS:CB	3:C:2027:HOH:O	2.61	0.49
1:C:269:GLU:N	1:C:270:PRO:CD	2.76	0.49
1:A:223:GLN:NE2	3:C:2019:HOH:O	2.46	0.48
1:D:217:GLU:OE2	1:D:220:ARG:NH1	2.46	0.48
1:A:383:GLY:O	1:A:386:ILE:CG1	2.61	0.48
1:C:285:LEU:O	1:D:209:ARG:NH1	2.47	0.48
1:B:28:SER:OG	1:B:52:SER:OG	2.32	0.48
1:B:217:GLU:OE1	1:B:220:ARG:NH2	2.46	0.47
1:C:373:ALA:C	1:C:374:ASP:OD1	2.52	0.47
1:C:31:ASN:N	1:C:43:GLN:OE1	2.48	0.46
1:D:70:GLU:CG	1:D:73:ARG:NH2	2.79	0.46
1:C:231:THR:CB	1:C:232:GLU:OE1	2.64	0.45
1:B:334:GLU:N	1:B:334:GLU:OE1	2.50	0.45
1:A:62:GLU:OE1	1:A:98:LYS:NZ	2.50	0.44
1:B:196:GLU:OE2	1:B:223:GLN:NE2	2.51	0.44
1:B:270:PRO:O	1:B:272:THR:N	2.50	0.44
1:D:34:THR:OG1	1:D:58:THR:O	2.35	0.44
1:D:171:HIS:NE2	1:D:210:ASP:OD2	2.50	0.44
1:C:326:TRP:CZ2	1:C:395:GLU:OE1	2.71	0.44
1:A:318:ARG:O	1:A:319:LEU:C	2.55	0.43
1:D:318:ARG:NH2	1:D:388:GLU:OE2	2.51	0.43
1:B:209:ARG:N	3:B:2018:HOH:O	2.51	0.43
1:D:90:PHE:CD1	1:D:90:PHE:C	2.91	0.43
1:D:206:SER:N	3:D:2012:HOH:O	2.52	0.43
1:B:373:ALA:O	1:B:375:GLY:N	2.52	0.43
1:D:101:LYS:CD	1:D:101:LYS:N	2.82	0.42
1:A:5:ARG:CZ	1:A:24:ILE:CD1	2.98	0.42
1:D:385:GLY:O	1:D:386:ILE:C	2.57	0.42
1:A:187:GLU:OE1	1:C:220:ARG:NH2	2.53	0.42
1:A:61:ASP:OD1	1:A:64:ALA:N	2.52	0.42
1:A:155:THR:OG1	1:B:300:CYS:O	2.38	0.42
1:C:56:ARG:CD	1:C:87:ASP:OD2	2.68	0.41
1:C:237:VAL:O	1:C:238:LYS:C	2.59	0.41
1:C:171:HIS:NE2	1:C:210:ASP:OD2	2.54	0.41
1:C:36:ASP:O	1:C:40:THR:N	2.54	0.41
1:A:366:GLU:O	1:A:368:LYS:N	2.53	0.41
1:A:220:ARG:NH2	1:C:187:GLU:OE1	2.54	0.41
1:C:385:GLY:O	1:C:386:ILE:C	2.59	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/406 (99%)	382 (95%)	18 (4%)	1 (0%)	56	79
1	B	390/406 (96%)	367 (94%)	18 (5%)	5 (1%)	18	29
1	C	386/406 (95%)	348 (90%)	35 (9%)	3 (1%)	27	46
1	D	389/406 (96%)	351 (90%)	30 (8%)	8 (2%)	11	16
All	All	1566/1624 (96%)	1448 (92%)	101 (6%)	17 (1%)	21	34

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	LYS
1	B	90	PHE
1	B	374	ASP
1	C	235	MET
1	D	90	PHE
1	D	382	LYS
1	D	403	ALA
1	C	91	ASN
1	B	367	PRO
1	B	382	LYS
1	D	92	GLY
1	D	196	GLU
1	D	386	ILE
1	D	125	HIS
1	D	301	GLY
1	B	299	GLY
1	C	113	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/325 (98%)	297 (93%)	23 (7%)	21	36
1	B	313/325 (96%)	276 (88%)	37 (12%)	8	14
1	C	313/325 (96%)	276 (88%)	37 (12%)	8	14
1	D	313/325 (96%)	268 (86%)	45 (14%)	5	8
All	All	1259/1300 (97%)	1117 (89%)	142 (11%)	9	15

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	78	GLU
1	A	81	GLU
1	A	84	LEU
1	A	96	LEU
1	A	110	ARG
1	A	118	ARG
1	A	122	LYS
1	A	145	ASN
1	A	149	LEU
1	A	258	THR
1	A	260	ARG
1	A	273	LYS
1	A	287	LEU
1	A	288	ARG
1	A	309	GLN
1	A	313	GLU
1	A	322	ARG
1	A	323	LEU
1	A	360	LEU
1	A	376	LYS
1	A	384	GLU
1	A	392	ARG
1	B	5	ARG
1	B	40	THR
1	B	57	LEU
1	B	60	ASN
1	B	84	LEU
1	B	90	PHE
1	B	96	LEU
1	B	97	ARG
1	B	101	LYS
1	B	110	ARG

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Mol	Chain	Res	Type
1	B	111	ILE
1	B	125	HIS
1	B	136	LEU
1	B	156	GLU
1	B	160	ARG
1	B	190	LEU
1	B	191	GLU
1	B	198	LYS
1	B	205	VAL
1	B	231	THR
1	B	232	GLU
1	B	238	LYS
1	B	252	LEU
1	B	263	LEU
1	B	272	THR
1	B	287	LEU
1	B	306	THR
1	B	310	GLU
1	B	320	LYS
1	B	345	VAL
1	B	374	ASP
1	B	376	LYS
1	B	381	LEU
1	B	386	ILE
1	B	391	LEU
1	B	392	ARG
1	B	401	ARG
1	C	4	MET
1	C	15	ARG
1	C	28	SER
1	C	53	GLU
1	C	57	LEU
1	C	58	THR
1	C	73	ARG
1	C	76	LEU
1	C	91	ASN
1	C	95	LEU
1	C	96	LEU
1	C	102	MET
1	C	104	GLU
1	C	115	THR
1	C	125	HIS

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	157	LEU
1	C	232	GLU
1	C	243	SER
1	C	247	LEU
1	C	252	LEU
1	C	262	SER
1	C	263	LEU
1	C	271	ARG
1	C	279	GLN
1	C	282	LEU
1	C	283	GLN
1	C	287	LEU
1	C	304	THR
1	C	310	GLU
1	C	314	GLU
1	C	318	ARG
1	C	360	LEU
1	C	374	ASP
1	C	376	LYS
1	C	396	ASP
1	C	405	LYS
1	D	13	VAL
1	D	26	VAL
1	D	31	ASN
1	D	35	ARG
1	D	40	THR
1	D	44	VAL
1	D	74	ARG
1	D	76	LEU
1	D	90	PHE
1	D	91	ASN
1	D	94	LEU
1	D	101	LYS
1	D	111	ILE
1	D	112	ASN
1	D	124	GLU
1	D	126	PHE
1	D	135	ASP
1	D	140	VAL
1	D	181	SER
1	D	187	GLU

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Mol	Chain	Res	Type
1	D	190	LEU
1	D	191	GLU
1	D	194	LEU
1	D	204	LYS
1	D	218	LEU
1	D	232	GLU
1	D	260	ARG
1	D	277	VAL
1	D	283	GLN
1	D	288	ARG
1	D	297	CYS
1	D	306	THR
1	D	310	GLU
1	D	316	SER
1	D	319	LEU
1	D	320	LYS
1	D	322	ARG
1	D	334	GLU
1	D	360	LEU
1	D	374	ASP
1	D	376	LYS
1	D	382	LYS
1	D	388	GLU
1	D	392	ARG
1	D	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	A	501	1	12,12,12	7.11	10 (83%)	0,24,24	0.00	-
2	SF4	B	501	1	12,12,12	6.99	11 (91%)	0,24,24	0.00	-
2	SF4	C	501	1	12,12,12	6.13	10 (83%)	0,24,24	0.00	-
2	SF4	D	501	1	12,12,12	7.52	11 (91%)	0,24,24	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	501	1	-	0/0/48/48	0/0/5/5
2	SF4	B	501	1	-	0/0/48/48	0/0/5/5
2	SF4	C	501	1	-	0/0/48/48	0/0/5/5
2	SF4	D	501	1	-	0/0/48/48	0/0/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	SF4	S2-FE3	-13.95	2.23	2.33
2	D	501	SF4	S1-FE3	-12.81	2.24	2.33
2	C	501	SF4	S2-FE1	-11.97	2.25	2.33
2	A	501	SF4	S2-FE4	-11.16	2.25	2.33
2	A	501	SF4	S3-FE1	-11.01	2.25	2.33
2	D	501	SF4	S1-FE2	-10.54	2.26	2.33
2	A	501	SF4	S3-FE2	-10.48	2.26	2.33
2	D	501	SF4	S3-FE1	-9.89	2.26	2.33
2	B	501	SF4	S2-FE1	-9.51	2.26	2.33
2	A	501	SF4	S2-FE1	-9.15	2.27	2.33
2	C	501	SF4	S3-FE1	-9.05	2.27	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	SF4	S4-FE2	-8.54	2.27	2.33
2	B	501	SF4	S1-FE4	-8.45	2.27	2.33
2	D	501	SF4	S3-FE2	-8.38	2.27	2.33
2	C	501	SF4	S3-FE4	-7.50	2.28	2.33
2	B	501	SF4	S3-FE4	-7.45	2.28	2.33
2	C	501	SF4	S2-FE3	-7.19	2.28	2.33
2	D	501	SF4	S4-FE1	-6.45	2.28	2.33
2	D	501	SF4	S4-FE3	-6.31	2.29	2.33
2	B	501	SF4	S3-FE2	-6.29	2.29	2.33
2	D	501	SF4	S2-FE4	-6.19	2.29	2.33
2	A	501	SF4	S4-FE3	-6.08	2.29	2.33
2	A	501	SF4	S3-FE4	-6.08	2.29	2.33
2	B	501	SF4	S3-FE1	-5.97	2.29	2.33
2	A	501	SF4	S1-FE3	-5.90	2.29	2.33
2	C	501	SF4	S3-FE2	-5.82	2.29	2.33
2	B	501	SF4	S1-FE2	-5.71	2.29	2.33
2	A	501	SF4	S4-FE1	-5.44	2.29	2.33
2	B	501	SF4	S4-FE1	-5.27	2.29	2.33
2	D	501	SF4	S2-FE3	-5.08	2.29	2.33
2	C	501	SF4	S2-FE4	4.73	2.36	2.33
2	C	501	SF4	S4-FE3	-4.63	2.30	2.33
2	A	501	SF4	S1-FE4	-4.28	2.30	2.33
2	B	501	SF4	S1-FE3	-4.21	2.30	2.33
2	C	501	SF4	S4-FE2	-3.93	2.30	2.33
2	B	501	SF4	S4-FE2	-3.87	2.30	2.33
2	C	501	SF4	S1-FE2	-3.48	2.30	2.33
2	D	501	SF4	S2-FE1	-3.28	2.31	2.33
2	A	501	SF4	S2-FE3	-2.76	2.31	2.33
2	C	501	SF4	S1-FE4	-2.60	2.31	2.33
2	D	501	SF4	S3-FE4	2.21	2.34	2.33
2	B	501	SF4	S2-FE4	2.15	2.34	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	403/406 (99%)	0.17	6 (1%) 70 72	41, 69, 118, 151	0
1	B	394/406 (97%)	0.33	16 (4%) 35 36	48, 79, 130, 164	0
1	C	392/406 (96%)	0.59	36 (9%) 9 8	48, 87, 171, 206	0
1	D	393/406 (96%)	0.50	31 (7%) 13 12	62, 93, 150, 243	0
All	All	1582/1624 (97%)	0.40	89 (5%) 24 24	41, 82, 146, 243	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	LEU	7.6
1	C	77	ALA	7.1
1	C	406	ALA	6.6
1	C	115	THR	6.1
1	C	39	ALA	5.5
1	D	59	VAL	4.8
1	D	319	LEU	4.8
1	D	405	LYS	4.5
1	D	406	ALA	4.5
1	C	76	LEU	4.3
1	C	101	LYS	4.2
1	C	381	LEU	4.0
1	D	404	PRO	3.9
1	C	405	LYS	3.7
1	C	75	LEU	3.6
1	C	73	ARG	3.6
1	C	79	GLY	3.6
1	B	91	ASN	3.5
1	B	266	SER	3.5
1	C	90	PHE	3.3
1	B	268	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	132	ILE	3.2
1	D	194	LEU	3.2
1	C	35	ARG	3.1
1	D	324	PRO	3.1
1	C	80	VAL	3.1
1	D	130	ILE	3.1
1	B	90	PHE	3.0
1	C	290	PHE	3.0
1	B	38	GLU	3.0
1	C	270	PRO	3.0
1	A	406	ALA	3.0
1	B	382	LYS	3.0
1	C	100	PRO	3.0
1	B	94	LEU	3.0
1	B	114	GLY	2.9
1	D	330	TYR	2.9
1	C	114	GLY	2.9
1	B	59	VAL	2.9
1	C	72	LYS	2.8
1	D	320	LYS	2.8
1	C	68	VAL	2.8
1	D	329	ARG	2.8
1	C	99	TYR	2.8
1	C	105	ALA	2.8
1	C	34	THR	2.8
1	D	332	GLY	2.8
1	D	77	ALA	2.7
1	B	267	PRO	2.7
1	C	269	GLU	2.7
1	D	321	GLU	2.6
1	D	323	LEU	2.6
1	D	378	LEU	2.6
1	D	290	PHE	2.6
1	C	111	ILE	2.6
1	D	325	GLU	2.6
1	B	76	LEU	2.5
1	D	90	PHE	2.5
1	A	267	PRO	2.5
1	C	84	LEU	2.5
1	C	88	PHE	2.4
1	B	405	LYS	2.4
1	D	403	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	384	GLU	2.3
1	B	363	ALA	2.3
1	A	268	LYS	2.3
1	D	39	ALA	2.3
1	D	368	LYS	2.3
1	D	189	ALA	2.3
1	C	382	LYS	2.3
1	C	64	ALA	2.3
1	D	381	LEU	2.2
1	A	380	ILE	2.2
1	B	265	PRO	2.2
1	C	404	PRO	2.2
1	B	96	LEU	2.1
1	C	102	MET	2.1
1	D	390	PHE	2.1
1	D	331	PRO	2.1
1	D	244	ALA	2.1
1	A	76	LEU	2.1
1	D	45	LEU	2.1
1	C	324	PRO	2.1
1	D	124	GLU	2.1
1	C	94	LEU	2.0
1	C	98	LYS	2.0
1	A	77	ALA	2.0
1	B	89	HIS	2.0
1	C	130	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SF4	D	501	8/8	0.17	2.01	60,63,67,68	0
2	SF4	A	501	8/8	0.17	1.23	72,77,81,82	0
2	SF4	B	501	8/8	0.16	0.57	62,65,68,69	0
2	SF4	C	501	8/8	0.15	0.53	65,67,70,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.