



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

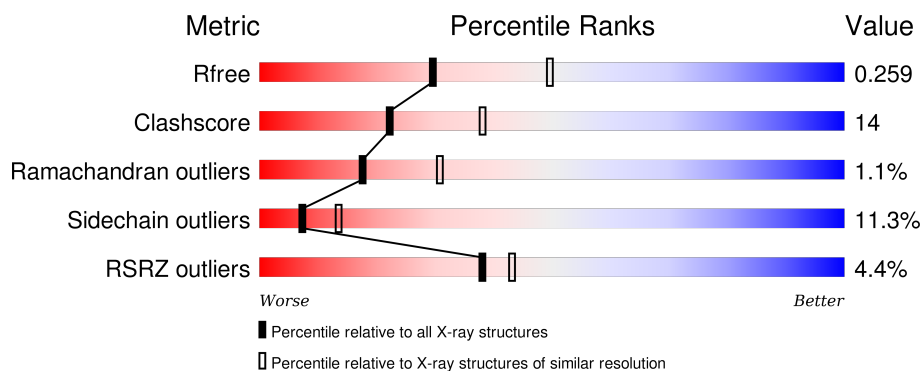
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 73%, yellow 73%, yellow 94%, orange 94%, orange 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 73% 21% </div> </div>
1	B	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 67%, yellow 67%, yellow 93%, orange 93%, orange 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 67% 26% </div> </div>
1	C	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 63%, yellow 63%, yellow 91%, orange 91%, orange 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 63% 28% 5% </div> </div>
1	D	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 60%, yellow 60%, yellow 92%, orange 92%, orange 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 60% 32% </div> </div>

2 Entry composition [i](#)

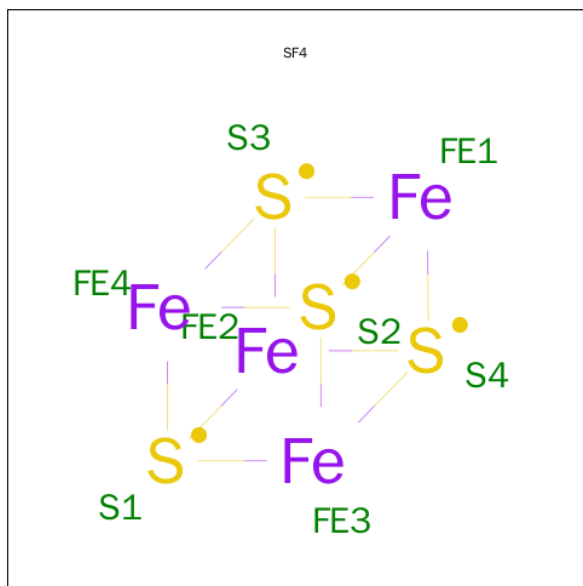
There are 3 unique types of molecules in this entry. The entry contains 12245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE 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 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

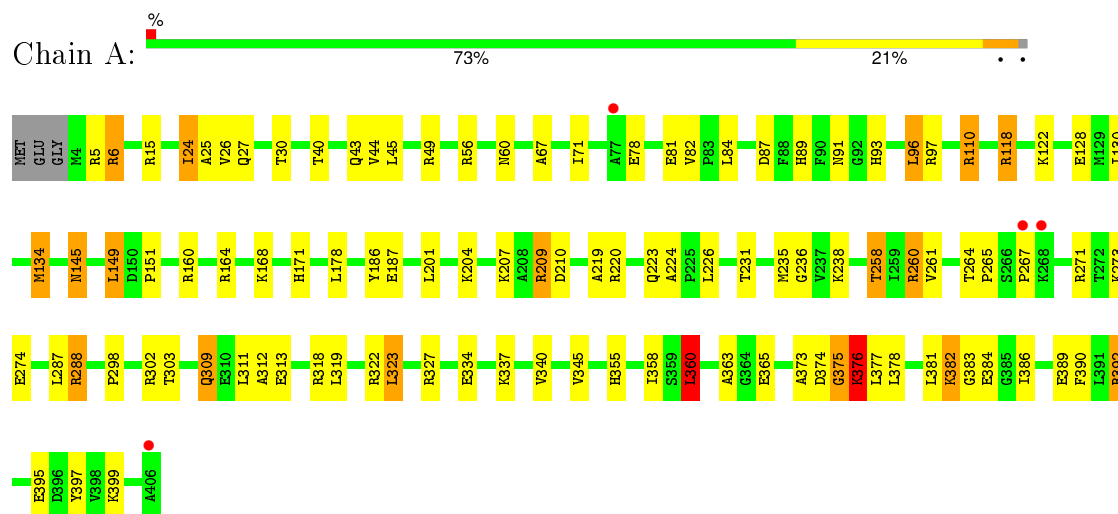
- Molecule 3 is water.

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

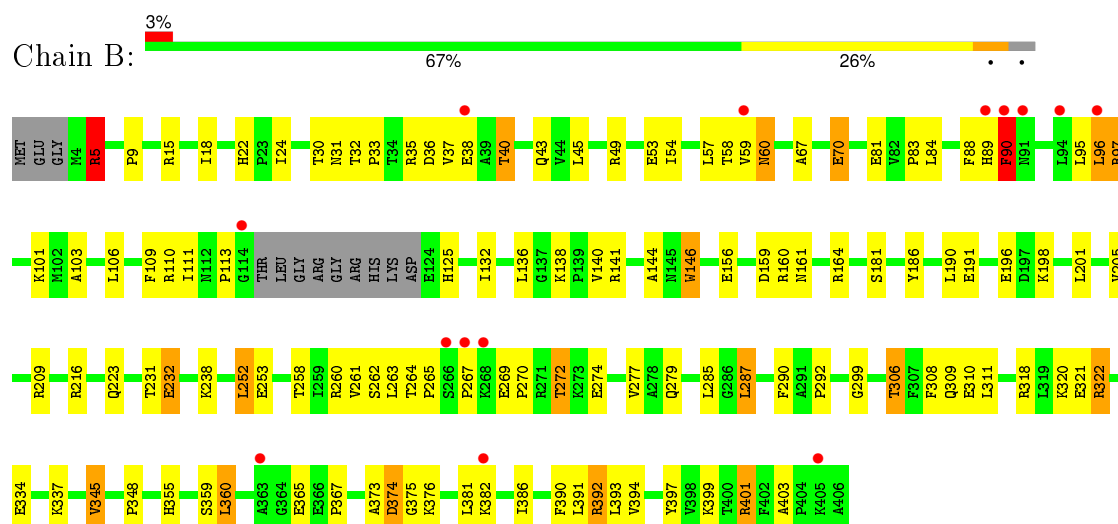
3 Residue-property plots

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-YL DIPHOSPHATE SYNTHASE

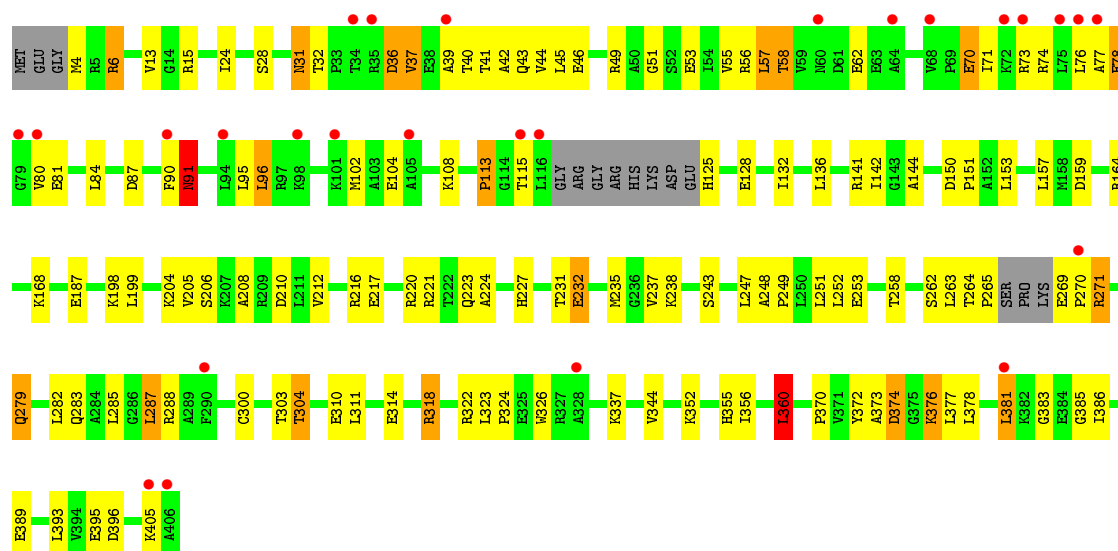


- Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE SYNTHASE

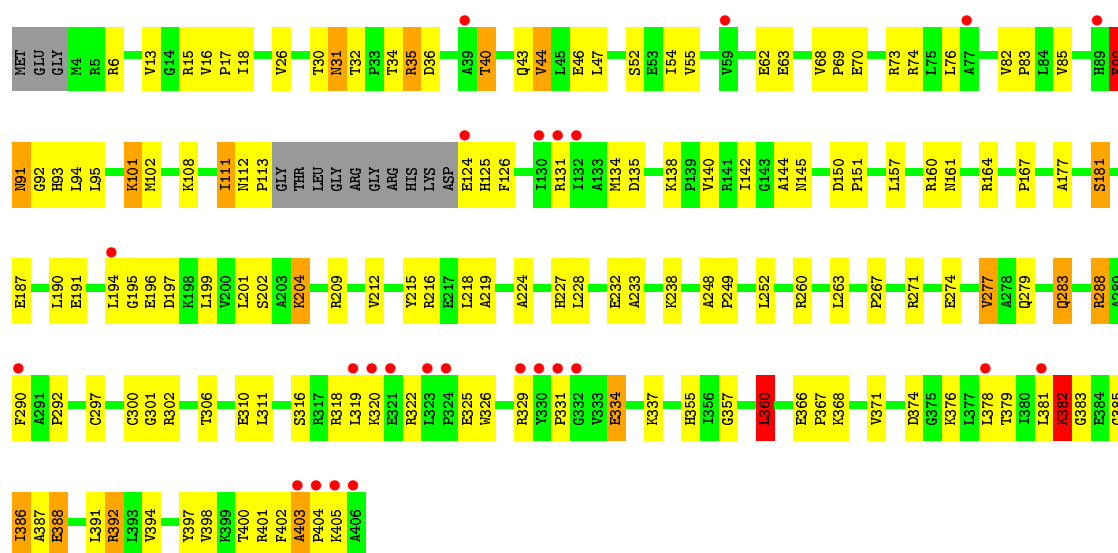


- Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE SYNTHASE





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



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 0.197 , 0.259	Depositor DCC
R_{free} test set	3608 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)	0.32 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical 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: 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 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	3077	0	3148	83	0
1	B	3005	0	3073	76	0
1	C	2995	0	3076	95	0
1	D	3001	0	3070	92	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	5	0
3	B	35	0	0	3	0
3	C	28	0	0	8	0
3	D	16	0	0	3	0
All	All	12245	0	12367	337	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 14.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HA	1:A:386:ILE:HD11	1.21	1.17
1:C:271:ARG:HH11	1:C:271:ARG:HG2	1.13	1.09
1:D:381:LEU:O	1:D:383:GLY:N	1.97	0.96
1:A:376:LYS:HB3	3:C:2027:HOH:O	1.66	0.96
1:A:337:LYS:H	1:A:355:HIS:HD2	1.09	0.94
1:B:90:PHE:HD1	1:B:90:PHE:H	1.19	0.91
1:A:383:GLY:O	1:A:386:ILE:HG13	1.69	0.91
1:C:223:GLN:NE2	3:C:2019:HOH:O	2.03	0.90
1:D:101:LYS:H	1:D:101:LYS:HD2	1.37	0.89
1:A:337:LYS:H	1:A:355:HIS:CD2	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HA	1:A:386:ILE:CD1	2.03	0.87
1:A:288:ARG:HH11	1:A:288:ARG:HG2	1.39	0.87
1:D:70:GLU:HG2	1:D:73:ARG:NH2	1.91	0.86
1:C:271:ARG:NH1	1:C:271:ARG:HG2	1.86	0.86
1:A:309:GLN:HA	1:A:309:GLN:HE21	1.40	0.85
1:C:352:LYS:HE3	1:D:167:PRO:HD2	1.60	0.84
1:A:235:MET:HG3	1:A:236:GLY:H	1.41	0.84
1:D:331:PRO:HD2	1:D:403:ALA:HA	1.60	0.83
1:C:337:LYS:H	1:C:355:HIS:CD2	1.97	0.83
1:D:403:ALA:HB1	1:D:404:PRO:HD2	1.61	0.83
1:C:90:PHE:O	1:C:91:ASN:HB3	1.76	0.83
1:D:337:LYS:H	1:D:355:HIS:HD2	1.27	0.83
1:C:205:VAL:HG11	1:C:210:ASP:HB2	1.60	0.82
1:A:235:MET:HG3	1:A:236:GLY:N	1.95	0.81
1:C:142:ILE:HD12	1:C:199:LEU:HD11	1.63	0.80
1:D:318:ARG:HG2	1:D:391:LEU:HD21	1.62	0.80
1:B:36:ASP:O	1:B:40:THR:HG23	1.83	0.79
1:D:279:GLN:HE21	1:D:288:ARG:HH21	1.30	0.78
1:D:91:ASN:HB2	3:D:2005:HOH:O	1.83	0.78
1:B:31:ASN:H	1:B:43:GLN:HE22	1.30	0.76
1:A:309:GLN:HA	1:A:309:GLN:NE2	1.99	0.76
1:D:70:GLU:HG2	1:D:73:ARG:HH22	1.50	0.74
1:A:235:MET:CG	1:A:236:GLY:H	2.01	0.74
1:C:374:ASP:OD2	3:C:2028:HOH:O	2.06	0.74
1:C:205:VAL:HG11	1:C:210:ASP:CB	2.17	0.73
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:A:288:ARG:NH1	1:A:288:ARG:HG2	2.01	0.72
1:B:306:THR:HG23	1:B:309:GLN:OE1	1.90	0.71
1:C:164:ARG:NH1	1:C:168:LYS:HD2	2.05	0.71
1:B:186:TYR:HB2	1:B:201:LEU:HD21	1.72	0.70
1:B:292:PRO:HD3	1:B:334:GLU:HA	1.73	0.70
1:A:302:ARG:NH1	1:B:159:ASP:OD1	2.25	0.70
1:B:232:GLU:HG2	1:B:262:SER:OG	1.92	0.70
1:C:31:ASN:HB2	1:C:271:ARG:HG3	1.73	0.70
1:C:383:GLY:O	1:C:386:ILE:HG13	1.91	0.69
1:B:261:VAL:HG11	1:B:277:VAL:HG22	1.75	0.69
1:C:337:LYS:H	1:C:355:HIS:HD2	1.36	0.69
1:A:219:ALA:O	3:C:2019:HOH:O	2.12	0.68
1:B:322:ARG:HG2	1:B:322:ARG:HH11	1.57	0.68
1:A:60:ASN:HD21	1:A:89:HIS:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:CYS:O	1:C:303:THR:HG22	1.93	0.68
1:C:42:ALA:O	1:C:45:LEU:HG	1.94	0.68
1:C:205:VAL:CG1	1:C:210:ASP:HB2	2.24	0.66
1:C:264:THR:HA	1:C:271:ARG:HH12	1.61	0.66
1:D:15:ARG:HD2	3:D:2004:HOH:O	1.95	0.65
1:B:106:LEU:O	1:B:138:LYS:HE3	1.96	0.65
1:A:145:ASN:ND2	3:A:2026:HOH:O	2.30	0.65
1:D:36:ASP:O	1:D:40:THR:HG23	1.97	0.65
1:B:401:ARG:CZ	1:B:401:ARG:HA	2.28	0.64
1:B:45:LEU:HD22	1:B:49:ARG:HH21	1.62	0.64
1:D:397:TYR:CZ	1:D:401:ARG:HG3	2.32	0.64
1:D:195:GLY:C	1:D:197:ASP:N	2.50	0.64
1:C:41:THR:HG22	1:C:71:ILE:HG23	1.80	0.63
1:C:159:ASP:OD1	1:D:302:ARG:NH1	2.31	0.63
1:A:6:ARG:NH2	1:A:226:LEU:HG	2.14	0.63
1:B:5:ARG:NH2	1:B:22:HIS:O	2.31	0.62
1:A:67:ALA:O	1:A:71:ILE:HG13	1.99	0.62
1:A:91:ASN:HD22	1:A:93:HIS:HE1	1.46	0.62
1:D:62:GLU:HG2	1:D:95:LEU:CD2	2.29	0.62
1:B:96:LEU:HD12	1:B:103:ALA:HB2	1.81	0.62
1:D:326:TRP:CH2	1:D:398:VAL:HG21	2.35	0.62
1:D:212:VAL:O	1:D:216:ARG:HG3	1.99	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:A:288:ARG:HH11	1:A:288:ARG:CG	2.12	0.61
1:C:217:GLU:CD	1:C:220:ARG:HH12	2.03	0.61
1:D:195:GLY:C	1:D:197:ASP:H	2.02	0.60
1:A:25:ALA:HB3	1:A:258:THR:HG22	1.82	0.60
1:B:31:ASN:N	1:B:43:GLN:HE22	1.99	0.60
1:A:309:GLN:CA	1:A:309:GLN:HE21	2.11	0.60
1:B:348:PRO:HD3	1:B:359:SER:OG	2.02	0.60
1:C:32:THR:HG21	1:C:39:ALA:O	2.00	0.60
1:C:6:ARG:NH2	1:C:224:ALA:O	2.24	0.60
1:D:62:GLU:HG2	1:D:95:LEU:HD21	1.84	0.60
1:C:24:ILE:HD13	1:C:251:LEU:HD22	1.83	0.60
1:B:30:THR:HA	1:B:43:GLN:NE2	2.16	0.59
1:D:382:LYS:HA	1:D:386:ILE:HD11	1.84	0.59
1:A:56:ARG:HD2	1:A:87:ASP:OD2	2.02	0.59
1:A:160:ARG:HD2	1:A:160:ARG:C	2.23	0.59
1:C:37:VAL:HA	1:C:40:THR:HG22	1.85	0.59
1:A:56:ARG:NH2	3:A:2009:HOH:O	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:O	1:B:40:THR:CG2	2.50	0.58
1:A:164:ARG:NH1	1:A:168:LYS:HD2	2.17	0.58
1:D:32:THR:OG1	1:D:40:THR:HB	2.03	0.58
1:A:97:ARG:HD3	1:A:128:GLU:OE2	2.04	0.58
1:C:56:ARG:HD2	1:C:87:ASP:OD2	2.03	0.58
1:D:36:ASP:O	1:D:40:THR:HG22	2.04	0.58
1:B:311:LEU:HD22	1:B:360:LEU:HD11	1.86	0.58
1:D:111:ILE:HD11	1:D:142:ILE:HG12	1.84	0.58
1:A:337:LYS:N	1:A:355:HIS:HD2	1.92	0.57
1:C:13:VAL:HG22	1:C:108:LYS:HD2	1.85	0.57
1:B:31:ASN:ND2	1:B:269:GLU:O	2.39	0.56
1:D:397:TYR:CE2	1:D:401:ARG:HG3	2.40	0.56
1:C:374:ASP:OD1	1:C:374:ASP:N	2.38	0.56
1:D:283:GLN:HG3	1:D:290:PHE:CD2	2.41	0.55
1:D:402:PHE:O	1:D:403:ALA:HB3	2.06	0.55
1:B:252:LEU:HD13	1:B:285:LEU:HD22	1.87	0.55
1:D:403:ALA:HB1	1:D:404:PRO:CD	2.35	0.55
1:C:41:THR:HG21	1:C:74:ARG:HD2	1.86	0.55
1:C:91:ASN:ND2	1:C:91:ASN:C	2.59	0.55
1:C:231:THR:O	1:C:232:GLU:HB3	2.06	0.55
1:D:113:PRO:HG2	1:D:144:ALA:HA	1.88	0.55
1:A:171:HIS:NE2	1:A:210:ASP:OD2	2.39	0.55
1:D:30:THR:HA	1:D:43:GLN:NE2	2.22	0.55
1:A:24:ILE:HD13	1:A:24:ILE:N	2.21	0.55
1:A:223:GLN:NE2	3:C:2018:HOH:O	2.41	0.54
1:C:326:TRP:HZ2	1:C:395:GLU:OE1	1.91	0.54
1:B:258:THR:HG21	3:B:2010:HOH:O	2.07	0.54
1:B:399:LYS:O	1:B:403:ALA:HB2	2.07	0.54
1:C:51:GLY:HA3	1:C:279:GLN:HE22	1.72	0.54
1:A:381:LEU:O	1:A:383:GLY:N	2.33	0.54
1:D:101:LYS:H	1:D:101:LYS:CD	2.15	0.54
1:B:181:SER:HB2	3:B:2013:HOH:O	2.08	0.53
1:C:205:VAL:CG1	1:C:206:SER:N	2.71	0.53
1:D:101:LYS:HD2	1:D:101:LYS:N	2.17	0.53
1:A:91:ASN:HD22	1:A:93:HIS:CE1	2.26	0.53
1:C:287:LEU:O	1:C:288:ARG:HG2	2.08	0.53
1:C:208:ALA:O	1:C:212:VAL:HG23	2.09	0.53
1:B:216:ARG:NH2	1:B:253:GLU:OE2	2.33	0.53
1:C:269:GLU:N	1:C:270:PRO:HD3	2.24	0.53
1:B:401:ARG:NE	1:B:401:ARG:HA	2.24	0.53
1:D:85:VAL:HG22	1:D:108:LYS:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:THR:O	1:D:44:VAL:HG12	2.09	0.53
1:C:265:PRO:HD3	1:C:271:ARG:HH12	1.74	0.53
1:B:9:PRO:HG3	1:B:196:GLU:HB3	1.90	0.53
1:A:382:LYS:CA	1:A:386:ILE:HD11	2.15	0.52
1:A:207:LYS:NZ	3:A:2043:HOH:O	2.42	0.52
1:D:402:PHE:O	1:D:403:ALA:CB	2.57	0.52
1:D:91:ASN:CB	3:D:2005:HOH:O	2.50	0.52
1:A:238:LYS:NZ	3:A:2050:HOH:O	2.42	0.52
1:C:231:THR:HB	1:C:232:GLU:OE1	2.09	0.52
1:B:337:LYS:H	1:B:355:HIS:CD2	2.28	0.52
1:B:90:PHE:N	1:B:90:PHE:CD1	2.68	0.51
1:C:217:GLU:OE2	1:C:220:ARG:NH1	2.38	0.51
1:A:238:LYS:HB2	1:A:238:LYS:NZ	2.24	0.51
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.10	0.51
1:A:311:LEU:HD23	1:A:360:LEU:HD11	1.92	0.51
1:D:215:TYR:CD2	1:D:228:LEU:HD23	2.45	0.51
1:C:128:GLU:O	1:C:132:ILE:HG13	2.11	0.51
1:B:18:ILE:HD11	1:B:54:ILE:HD11	1.92	0.51
1:B:345:VAL:HG22	1:B:365:GLU:OE2	2.11	0.51
1:D:6:ARG:NH2	1:D:224:ALA:O	2.44	0.51
1:D:31:ASN:H	1:D:43:GLN:HE22	1.58	0.51
1:D:248:ALA:HB3	1:D:249:PRO:HD3	1.93	0.51
1:D:68:VAL:HB	1:D:69:PRO:HD3	1.92	0.51
1:B:308:PHE:HA	1:B:360:LEU:HD13	1.92	0.51
1:A:389:GLU:HA	1:A:392:ARG:HH21	1.75	0.51
1:B:15:ARG:HG3	1:B:81:GLU:OE1	2.10	0.50
1:A:271:ARG:O	1:A:274:GLU:HG3	2.11	0.50
1:B:5:ARG:NH2	1:B:24:ILE:HG13	2.26	0.50
1:A:373:ALA:N	1:A:375:GLY:O	2.39	0.50
1:D:279:GLN:NE2	1:D:288:ARG:HH21	2.05	0.50
1:C:381:LEU:O	1:C:383:GLY:N	2.40	0.50
1:D:325:GLU:O	1:D:329:ARG:HB2	2.11	0.50
1:D:161:ASN:HA	1:D:164:ARG:HD2	1.94	0.50
1:C:57:LEU:HD21	1:C:84:LEU:HD23	1.94	0.50
1:D:34:THR:HA	1:D:40:THR:HG21	1.94	0.50
1:D:113:PRO:HD3	1:D:142:ILE:HG23	1.94	0.50
1:D:233:ALA:O	1:D:263:LEU:HA	2.11	0.49
1:D:357:GLY:O	1:D:371:VAL:HA	2.12	0.49
1:C:204:LYS:HE3	3:C:2012:HOH:O	2.11	0.49
1:B:252:LEU:CD1	1:B:285:LEU:HD22	2.41	0.49
1:C:56:ARG:HE	1:C:141:ARG:HH22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PHE:HA	1:B:393:LEU:HD12	1.94	0.49
1:C:370:PRO:HB3	1:C:376:LYS:NZ	2.27	0.49
1:B:161:ASN:HA	1:B:164:ARG:HD2	1.94	0.49
1:A:260:ARG:HG3	1:A:261:VAL:N	2.27	0.49
1:C:269:GLU:N	1:C:270:PRO:CD	2.76	0.49
1:B:390:PHE:O	1:B:394:VAL:HG23	2.12	0.49
1:A:395:GLU:O	1:A:399:LYS:HG3	2.12	0.49
1:D:367:PRO:O	1:D:382:LYS:HB2	2.13	0.49
1:A:149:LEU:O	1:A:151:PRO:HD3	2.13	0.49
1:A:15:ARG:HG3	3:A:2013:HOH:O	2.12	0.49
1:A:30:THR:HA	1:A:43:GLN:OE1	2.12	0.48
1:B:58:THR:HG22	1:B:60:ASN:HB2	1.95	0.48
1:D:382:LYS:HA	1:D:386:ILE:CD1	2.43	0.48
1:A:204:LYS:HE3	1:A:231:THR:HG21	1.95	0.48
1:C:271:ARG:CG	1:C:271:ARG:HH11	2.00	0.48
1:A:223:GLN:NE2	3:C:2019:HOH:O	2.46	0.48
1:C:81:GLU:O	1:C:81:GLU:HG3	2.13	0.48
1:A:377:LEU:O	1:A:378:LEU:HB3	2.14	0.48
1:D:145:ASN:HB2	1:D:204:LYS:HE3	1.96	0.48
1:D:47:LEU:O	1:D:52:SER:HB3	2.14	0.48
1:C:389:GLU:O	1:C:393:LEU:HG	2.14	0.48
1:C:285:LEU:O	1:D:209:ARG:NH1	2.47	0.48
1:C:356:ILE:HA	1:C:372:TYR:O	2.13	0.48
1:D:283:GLN:HG3	1:D:290:PHE:HD2	1.79	0.48
1:C:216:ARG:NH2	1:C:253:GLU:OE2	2.45	0.48
1:A:223:GLN:HE22	1:C:223:GLN:HE22	1.60	0.47
1:C:142:ILE:HD12	1:C:199:LEU:CD1	2.39	0.47
1:C:373:ALA:C	1:C:374:ASP:OD1	2.52	0.47
1:B:308:PHE:CZ	1:B:309:GLN:HG3	2.49	0.47
1:D:378:LEU:HG	1:D:379:THR:H	1.78	0.47
1:C:37:VAL:HA	1:C:40:THR:CG2	2.44	0.47
1:B:232:GLU:HG2	1:B:262:SER:HG	1.78	0.47
1:D:311:LEU:HD23	1:D:360:LEU:HD11	1.96	0.47
1:C:37:VAL:HG11	1:C:70:GLU:HG2	1.97	0.47
1:A:376:LYS:HG3	1:A:376:LYS:O	2.05	0.47
1:C:37:VAL:HG13	1:C:71:ILE:HG13	1.96	0.47
1:D:382:LYS:HG2	1:D:386:ILE:CD1	2.45	0.46
1:D:142:ILE:CD1	1:D:199:LEU:HD11	2.45	0.46
1:C:150:ASP:HB3	1:C:153:LEU:CB	2.45	0.46
1:B:90:PHE:N	1:B:90:PHE:HD1	1.99	0.46
1:D:331:PRO:HD2	1:D:403:ALA:CA	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:O	1:C:40:THR:HG22	2.15	0.46
1:B:89:HIS:HB3	1:B:90:PHE:HD1	1.79	0.46
1:A:40:THR:O	1:A:44:VAL:HG23	2.15	0.46
1:A:220:ARG:NH1	1:C:187:GLU:OE2	2.42	0.46
1:C:31:ASN:N	1:C:43:GLN:OE1	2.48	0.46
1:A:45:LEU:O	1:A:49:ARG:HG3	2.16	0.46
1:C:205:VAL:HG12	1:C:206:SER:N	2.31	0.46
1:A:130:ILE:O	1:A:134:MET:HG3	2.16	0.46
1:A:345:VAL:HG23	1:A:365:GLU:OE2	2.16	0.46
1:A:358:ILE:HB	1:A:390:PHE:CE1	2.51	0.46
1:B:392:ARG:HH11	1:B:392:ARG:HG3	1.81	0.46
1:C:318:ARG:O	1:C:322:ARG:HG2	2.16	0.45
1:D:292:PRO:HD3	1:D:334:GLU:HA	1.98	0.45
1:D:394:VAL:O	1:D:398:VAL:HG23	2.16	0.45
1:D:68:VAL:HB	1:D:102:MET:HG2	1.97	0.45
1:D:201:LEU:HD23	1:D:202:SER:N	2.31	0.45
1:A:6:ARG:NH2	1:A:224:ALA:O	2.40	0.45
1:D:157:LEU:HD22	1:D:160:ARG:NH2	2.31	0.45
1:C:265:PRO:HD3	1:C:271:ARG:NH1	2.31	0.45
1:D:150:ASP:HA	1:D:151:PRO:HD2	1.72	0.45
1:A:382:LYS:HG2	1:A:386:ILE:HD12	1.98	0.45
1:C:231:THR:CB	1:C:232:GLU:OE1	2.64	0.45
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.99	0.45
1:B:109:PHE:HB2	1:B:140:VAL:HG22	1.99	0.45
1:D:274:GLU:HA	1:D:277:VAL:HG13	1.98	0.45
1:B:59:VAL:HG12	1:B:95:LEU:HD23	1.98	0.45
1:C:74:ARG:O	1:C:78:GLU:N	2.45	0.44
1:D:44:VAL:HB	1:D:55:VAL:HG11	1.99	0.44
1:B:209:ARG:HB2	3:B:2018:HOH:O	2.16	0.44
1:D:177:ALA:O	1:D:181:SER:HB2	2.18	0.44
1:B:392:ARG:NH1	1:B:392:ARG:HG3	2.33	0.44
1:B:59:VAL:HB	1:B:88:PHE:CE1	2.53	0.44
1:C:323:LEU:HB3	1:C:324:PRO:HD3	1.99	0.44
1:C:344:VAL:HG13	1:C:370:PRO:HG2	2.00	0.44
1:B:270:PRO:O	1:B:272:THR:N	2.50	0.44
1:C:326:TRP:CZ2	1:C:395:GLU:OE1	2.71	0.44
1:B:53:GLU:O	1:B:83:PRO:HD2	2.18	0.44
1:A:318:ARG:O	1:A:319:LEU:C	2.55	0.43
1:D:90:PHE:CD1	1:D:90:PHE:C	2.91	0.43
1:B:31:ASN:H	1:B:43:GLN:NE2	2.08	0.43
1:D:18:ILE:HD11	1:D:54:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HB3	1:D:63:GLU:HG3	1.99	0.43
1:C:205:VAL:HG11	1:C:210:ASP:HB3	1.99	0.43
1:B:322:ARG:HG2	1:B:322:ARG:NH1	2.28	0.43
1:B:24:ILE:HD12	1:B:287:LEU:HG	1.99	0.43
1:D:31:ASN:C	1:D:31:ASN:HD22	2.22	0.43
1:C:376:LYS:HE2	1:C:376:LYS:HB2	1.50	0.43
1:D:271:ARG:O	1:D:274:GLU:HG2	2.19	0.43
1:A:355:HIS:HB3	1:A:397:TYR:CE1	2.54	0.43
1:D:400:THR:HG22	1:D:401:ARG:NH1	2.33	0.43
1:D:113:PRO:HD3	1:D:142:ILE:CG2	2.48	0.43
1:D:387:ALA:O	1:D:391:LEU:HB2	2.19	0.43
1:C:45:LEU:HD12	1:C:46:GLU:N	2.34	0.43
1:B:373:ALA:O	1:B:375:GLY:N	2.52	0.43
1:D:93:HIS:CD2	1:D:93:HIS:H	2.36	0.42
1:B:397:TYR:O	1:B:401:ARG:HB2	2.18	0.42
1:C:227:HIS:CD2	1:C:258:THR:HG21	2.53	0.42
1:B:113:PRO:HG3	1:B:144:ALA:HA	2.01	0.42
1:B:232:GLU:HA	1:B:262:SER:OG	2.20	0.42
1:D:385:GLY:O	1:D:386:ILE:C	2.57	0.42
1:A:5:ARG:CZ	1:A:24:ILE:CD1	2.98	0.42
1:C:377:LEU:O	1:C:378:LEU:HB3	2.19	0.42
1:B:33:PRO:HB3	1:B:35:ARG:HH21	1.84	0.42
1:A:96:LEU:HA	1:A:96:LEU:HD12	1.86	0.42
1:A:334:GLU:CD	1:A:334:GLU:H	2.22	0.42
1:C:56:ARG:NE	1:C:141:ARG:HH22	2.18	0.42
1:B:264:THR:HA	1:B:265:PRO:HD3	1.94	0.42
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.91	0.42
1:A:303:THR:HA	1:A:363:ALA:H	1.85	0.42
1:A:25:ALA:HB3	1:A:258:THR:CG2	2.49	0.42
1:C:150:ASP:HB3	1:C:153:LEU:HB2	2.02	0.42
1:A:82:VAL:O	1:A:82:VAL:HG13	2.19	0.42
1:A:118:ARG:HG3	1:A:118:ARG:O	2.20	0.42
1:B:196:GLU:OE2	1:B:223:GLN:NE2	2.51	0.41
1:A:264:THR:HA	1:A:265:PRO:HD3	1.98	0.41
1:C:91:ASN:HD22	1:C:91:ASN:C	2.23	0.41
1:B:32:THR:OG1	1:B:40:THR:HB	2.20	0.41
1:C:78:GLU:C	1:C:80:VAL:H	2.24	0.41
1:D:43:GLN:HA	1:D:46:GLU:HG2	2.02	0.41
1:B:318:ARG:HA	1:B:321:GLU:HG2	2.02	0.41
1:A:26:VAL:HG12	1:A:27:GLN:N	2.35	0.41
1:C:24:ILE:HD12	1:C:287:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HA	1:C:87:ASP:HB3	2.02	0.41
1:A:238:LYS:HB2	1:A:238:LYS:HZ2	1.84	0.41
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.87	0.41
1:C:237:VAL:O	1:C:238:LYS:C	2.59	0.41
1:C:205:VAL:CG1	1:C:210:ASP:CB	2.91	0.41
1:D:388:GLU:O	1:D:392:ARG:HD3	2.21	0.41
1:C:56:ARG:CD	1:C:87:ASP:OD2	2.68	0.41
1:B:37:VAL:HG22	1:B:67:ALA:HB1	2.02	0.41
1:A:327:ARG:HG3	1:A:327:ARG:HH11	1.85	0.41
1:B:261:VAL:HG11	1:B:277:VAL:CG2	2.47	0.41
1:D:366:GLU:O	1:D:368:LYS:N	2.44	0.41
1:D:238:LYS:HE3	1:D:238:LYS:HB2	1.85	0.41
1:A:298:PRO:HB2	1:B:146:TRP:CH2	2.56	0.41
1:A:91:ASN:HA	1:A:93:HIS:CE1	2.55	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.88	0.41
1:B:60:ASN:HD21	1:B:89:HIS:CG	2.38	0.41
1:A:209:ARG:HH11	1:A:209:ARG:HD2	1.69	0.41
1:D:337:LYS:H	1:D:355:HIS:CD2	2.19	0.41
1:C:311:LEU:HD23	1:C:360:LEU:HD11	2.01	0.41
1:D:16:VAL:HA	1:D:17:PRO:HD2	1.91	0.41
1:B:38:GLU:HA	1:B:38:GLU:OE1	2.20	0.41
1:A:312:ALA:HB2	1:A:340:VAL:HB	2.02	0.41
1:C:385:GLY:O	1:C:386:ILE:C	2.59	0.41
1:A:160:ARG:HD2	1:A:160:ARG:O	2.21	0.41
1:D:138:LYS:HD3	1:D:138:LYS:HA	1.86	0.41
1:C:113:PRO:HG2	1:C:144:ALA:HA	2.03	0.41
1:B:96:LEU:HD12	1:B:103:ALA:CB	2.48	0.40
1:D:202:SER:HB3	1:D:227:HIS:HB3	2.03	0.40
1:B:109:PHE:O	1:B:140:VAL:HA	2.21	0.40
1:A:186:TYR:HB2	1:A:201:LEU:HD21	2.03	0.40
1:C:44:VAL:HG22	1:C:55:VAL:HG11	2.02	0.40
1:B:97:ARG:NH1	1:B:132:ILE:HG12	2.37	0.40
1:B:279:GLN:HB3	1:B:290:PHE:HZ	1.86	0.40
1:C:198:LYS:HA	1:C:198:LYS:HD3	1.86	0.40
1:D:82:VAL:HA	1:D:83:PRO:HD2	1.93	0.40
1:C:90:PHE:O	1:C:91:ASN:CB	2.56	0.40
1:A:187:GLU:OE1	1:C:220:ARG:NH2	2.53	0.40
1:C:150:ASP:HA	1:C:151:PRO:HD2	1.96	0.40
1:D:131:ARG:O	1:D:134:MET:HG2	2.22	0.40
1:B:260:ARG:NH2	1:B:274:GLU:OE2	2.45	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	401/406 (99%)	382 (95%)	18 (4%)	1 (0%)	52	75
1	B	390/406 (96%)	367 (94%)	18 (5%)	5 (1%)	15	26
1	C	386/406 (95%)	348 (90%)	35 (9%)	3 (1%)	24	41
1	D	389/406 (96%)	351 (90%)	30 (8%)	8 (2%)	9	14
All	All	1566/1624 (96%)	1448 (92%)	101 (6%)	17 (1%)	17	31

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 [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	320/325 (98%)	297 (93%)	23 (7%)	18	33
1	B	313/325 (96%)	276 (88%)	37 (12%)	6	12
1	C	313/325 (96%)	276 (88%)	37 (12%)	6	12
1	D	313/325 (96%)	268 (86%)	45 (14%)	4	7
All	All	1259/1300 (97%)	1117 (89%)	142 (11%)	7	13

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

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Mol	Chain	Res	Type
1	B	90	PHE
1	B	96	LEU
1	B	97	ARG
1	B	101	LYS
1	B	110	ARG
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

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Mol	Chain	Res	Type
1	C	96	LEU
1	C	102	MET
1	C	104	GLU
1	C	115	THR
1	C	125	HIS
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

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Mol	Chain	Res	Type
1	D	126	PHE
1	D	135	ASP
1	D	140	VAL
1	D	181	SER
1	D	187	GLU
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. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	91	ASN
1	A	93	HIS
1	A	125	HIS
1	A	145	ASN
1	A	223	GLN
1	A	279	GLN
1	A	309	GLN

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Mol	Chain	Res	Type
1	A	346	ASN
1	A	355	HIS
1	B	43	GLN
1	B	60	ASN
1	B	346	ASN
1	B	355	HIS
1	C	91	ASN
1	C	279	GLN
1	C	346	ASN
1	C	355	HIS
1	D	27	GLN
1	D	31	ASN
1	D	43	GLN
1	D	93	HIS
1	D	112	ASN
1	D	145	ASN
1	D	279	GLN
1	D	283	GLN
1	D	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	501	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	D	501	1	0,12,12	0.00	-	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	0/6/5/5
2	SF4	B	501	1	-	0/0/48/48	0/6/5/5
2	SF4	C	501	1	-	0/0/48/48	0/6/5/5
2	SF4	D	501	1	-	0/0/48/48	0/6/5/5

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.

No monomer is involved in short contacts.

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	403/406 (99%)	0.03	4 (0%) 84 86	41, 69, 118, 151	0
1	B	394/406 (97%)	0.19	14 (3%) 46 51	48, 79, 130, 164	0
1	C	392/406 (96%)	0.46	26 (6%) 22 24	48, 87, 171, 206	0
1	D	393/406 (96%)	0.33	25 (6%) 23 25	62, 93, 150, 243	0
All	All	1582/1624 (97%)	0.25	69 (4%) 38 43	41, 82, 146, 243	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	LEU	8.6
1	C	77	ALA	6.7
1	C	406	ALA	6.6
1	C	115	THR	6.4
1	C	39	ALA	6.1
1	D	406	ALA	5.1
1	D	405	LYS	4.4
1	C	90	PHE	4.2
1	D	404	PRO	4.1
1	D	59	VAL	4.0
1	B	90	PHE	3.7
1	B	91	ASN	3.6
1	C	79	GLY	3.5
1	C	73	ARG	3.5
1	C	75	LEU	3.4
1	C	101	LYS	3.3
1	B	114	GLY	3.2
1	D	319	LEU	3.2
1	B	266	SER	3.2
1	C	381	LEU	3.1
1	C	270	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	35	ARG	3.0
1	B	38	GLU	3.0
1	C	72	LYS	3.0
1	C	76	LEU	3.0
1	B	59	VAL	3.0
1	D	132	ILE	2.9
1	D	403	ALA	2.9
1	C	405	LYS	2.8
1	D	321	GLU	2.8
1	A	267	PRO	2.8
1	C	80	VAL	2.7
1	D	329	ARG	2.7
1	D	124	GLU	2.7
1	A	406	ALA	2.7
1	C	105	ALA	2.7
1	D	77	ALA	2.7
1	C	290	PHE	2.7
1	D	290	PHE	2.6
1	D	332	GLY	2.6
1	D	330	TYR	2.6
1	D	130	ILE	2.6
1	C	34	THR	2.6
1	D	194	LEU	2.5
1	B	267	PRO	2.5
1	D	324	PRO	2.5
1	D	381	LEU	2.5
1	C	64	ALA	2.5
1	B	268	LYS	2.4
1	B	363	ALA	2.4
1	B	382	LYS	2.3
1	D	378	LEU	2.3
1	C	60	ASN	2.3
1	B	96	LEU	2.2
1	B	89	HIS	2.2
1	C	98	LYS	2.2
1	C	68	VAL	2.2
1	B	405	LYS	2.2
1	D	320	LYS	2.2
1	D	323	LEU	2.1
1	C	94	LEU	2.1
1	D	89	HIS	2.1
1	D	331	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	77	ALA	2.1
1	C	328	ALA	2.1
1	D	39	ALA	2.1
1	B	94	LEU	2.1
1	D	131	ARG	2.0
1	A	268	LYS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SF4	D	501	8/8	0.99	0.16	1.29	60,63,67,68	0
2	SF4	A	501	8/8	0.99	0.15	0.54	72,77,81,82	0
2	SF4	C	501	8/8	1.00	0.14	-0.00	65,67,70,77	0
2	SF4	B	501	8/8	0.99	0.15	-0.02	62,65,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.