



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 2Y0F / pdb_00002y0f
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

<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

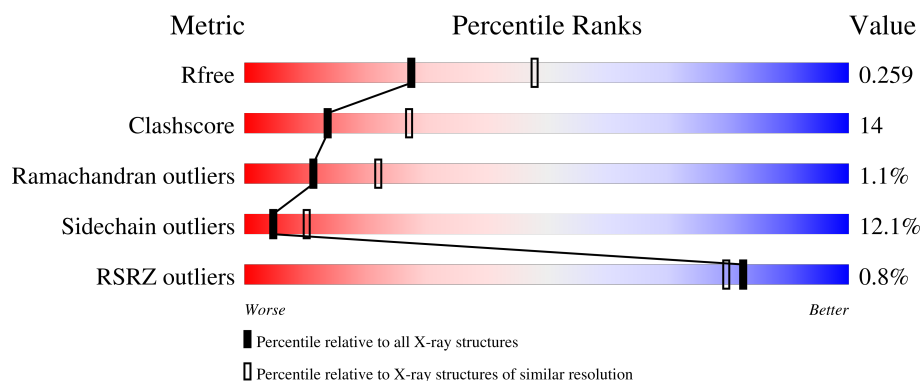
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	406	 72% 23% . .
1	B	406	 65% 27% 5% . .
1	C	406	 60% 32% . . .
1	D	406	 58% 31% 7% .

2 Entry composition [i](#)

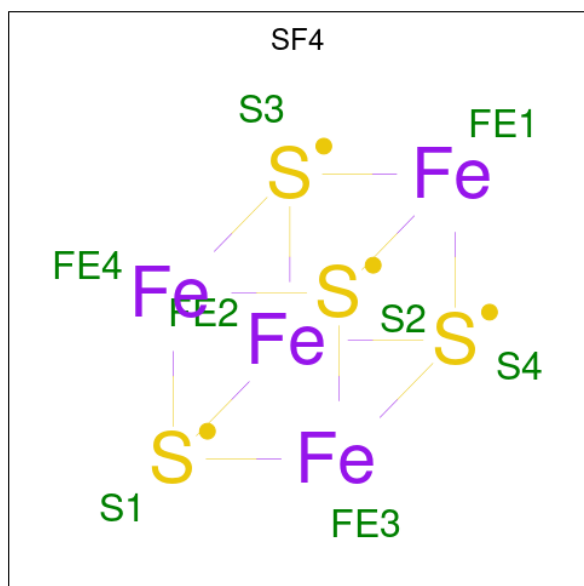
There are 3 unique types of molecules in this entry. The entry contains 12245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

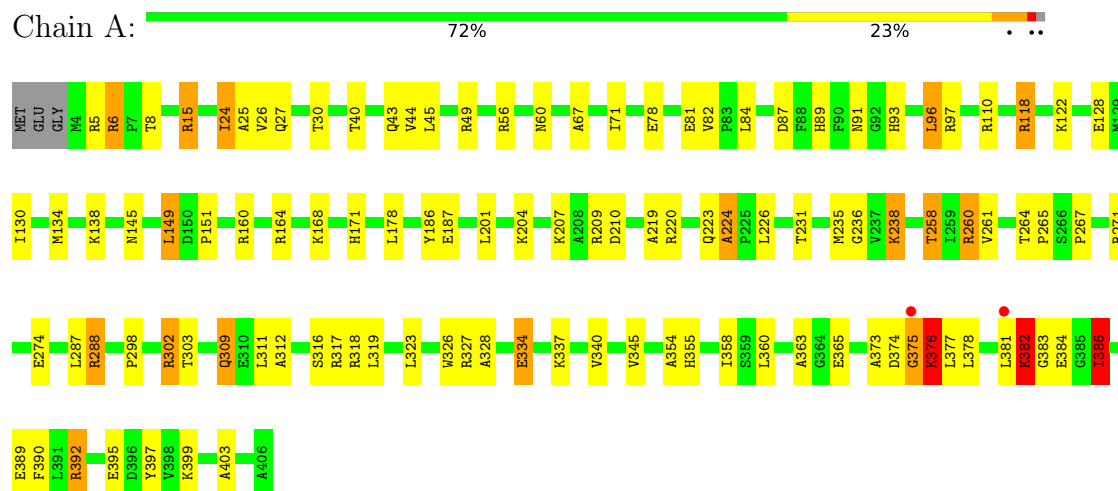
- Molecule 3 is water.

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		

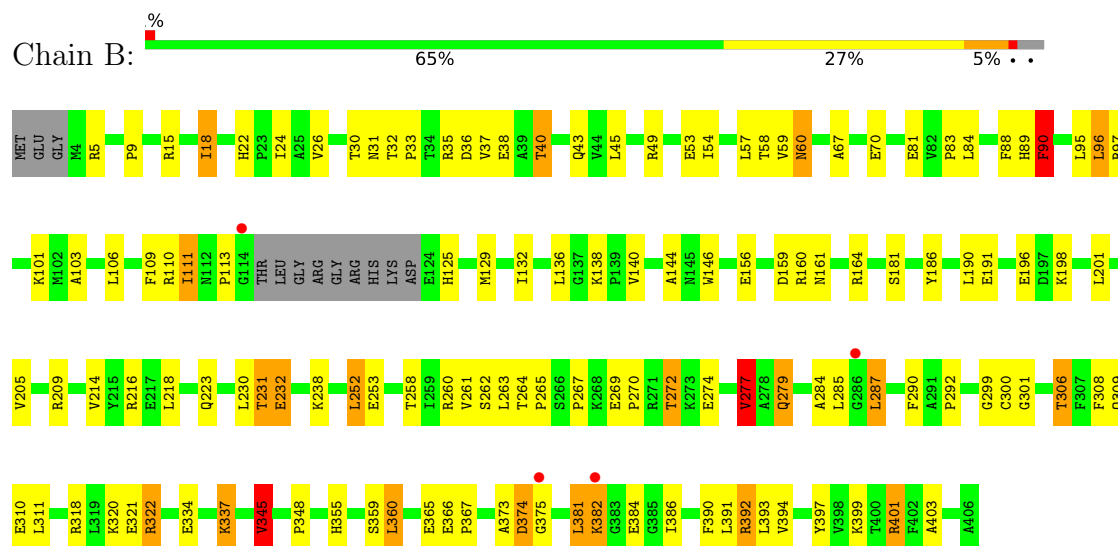
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE SYNTHASE

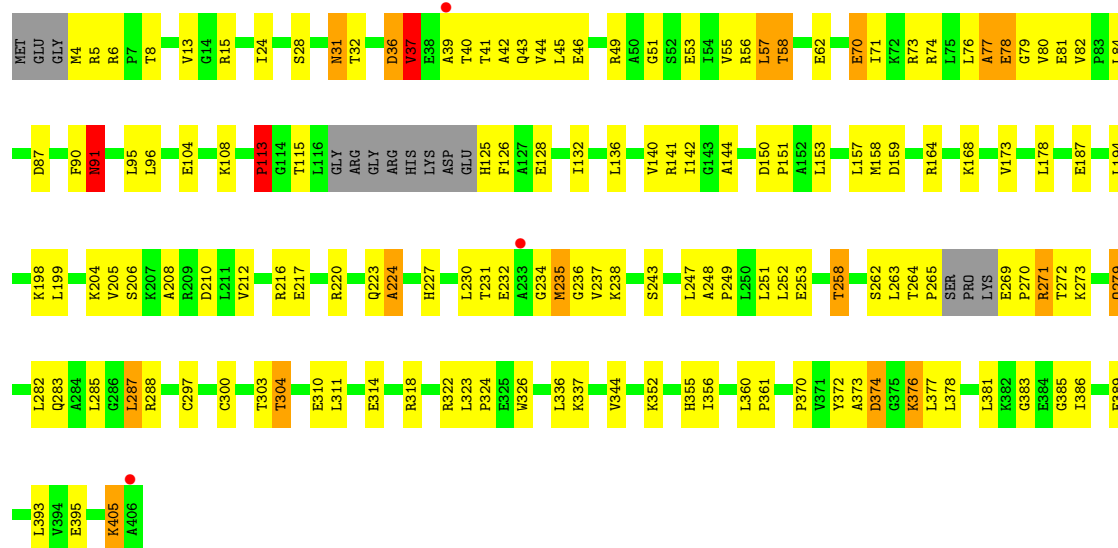


• Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE SYNTHASE

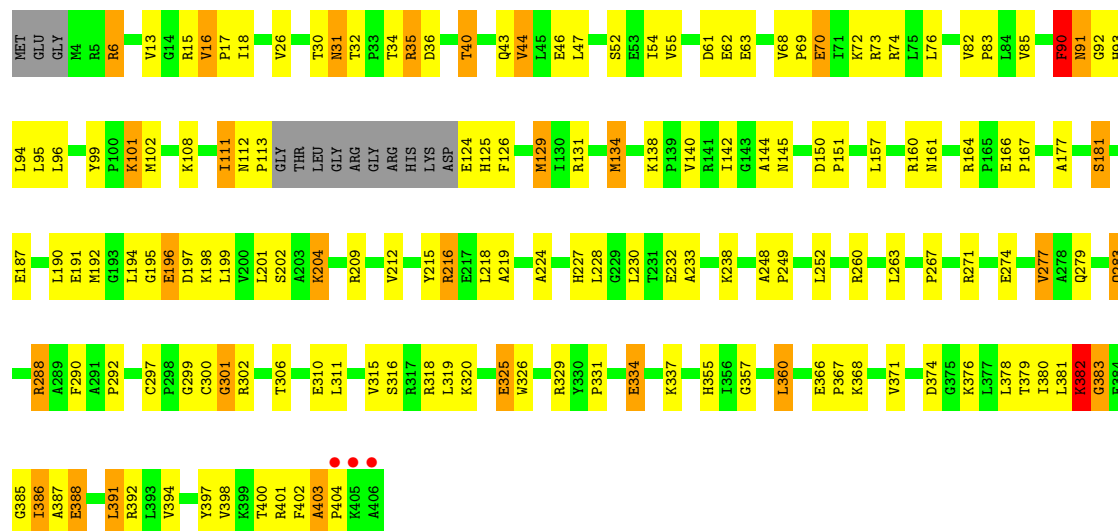


• Molecule 1: 4-HYDROXY-3-METHYLBUT-2-EN-1-YL DIPHOSPHATE SYNTHASE





• 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 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.50) 96.0 (20.00-2.50)	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	3609 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	1.09	4/3134 (0.1%)	1.27	17/4245 (0.4%)
1	B	0.97	3/3060 (0.1%)	1.18	13/4146 (0.3%)
1	C	1.23	14/3049 (0.5%)	1.19	14/4130 (0.3%)
1	D	0.89	1/3056 (0.0%)	1.16	13/4141 (0.3%)
All	All	1.05	22/12299 (0.2%)	1.20	57/16662 (0.3%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77	ALA	C-N	18.54	1.59	1.33
1	C	77	ALA	C-O	16.90	1.44	1.24
1	C	78	GLU	C-N	14.04	1.53	1.33
1	C	37	VAL	CA-CB	12.65	1.69	1.54
1	A	375	GLY	N-CA	12.35	1.59	1.45
1	C	78	GLU	CD-OE1	8.81	1.42	1.25
1	C	70	GLU	CD-OE1	8.67	1.41	1.25
1	C	36	ASP	C-O	8.52	1.35	1.23
1	A	375	GLY	CA-C	7.67	1.60	1.52
1	C	70	GLU	CD-OE2	7.39	1.39	1.25
1	A	376	LYS	N-CA	7.38	1.55	1.46
1	A	376	LYS	CA-C	6.63	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	VAL	CA-C	6.39	1.60	1.52
1	B	277	VAL	CA-CB	6.03	1.62	1.54
1	C	36	ASP	C-N	5.89	1.41	1.34
1	C	62	GLU	C-O	5.77	1.30	1.24
1	C	37	VAL	N-CA	-5.75	1.39	1.46
1	D	16	VAL	CA-C	5.37	1.58	1.52
1	B	218	LEU	N-CA	5.21	1.52	1.46
1	C	49	ARG	NE-CZ	5.16	1.38	1.33
1	B	26	VAL	CA-CB	-5.11	1.48	1.54
1	C	37	VAL	CB-CG2	-5.03	1.35	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	CA-C-N	-12.34	107.39	119.85
1	A	6	ARG	C-N-CA	-12.34	107.39	119.85
1	A	376	LYS	N-CA-C	11.85	127.80	108.96
1	A	8	THR	CA-C-N	-10.40	109.85	120.98
1	A	8	THR	C-N-CA	-10.40	109.85	120.98
1	B	384	GLU	N-CA-C	-9.68	99.59	111.40
1	C	31	ASN	N-CA-C	-9.37	102.94	114.75
1	D	6	ARG	CA-C-N	-8.36	110.68	120.13
1	D	6	ARG	C-N-CA	-8.36	110.68	120.13
1	D	267	PRO	N-CA-CB	8.21	110.48	103.25
1	C	297	CYS	CA-C-N	7.91	127.62	119.56
1	C	297	CYS	C-N-CA	7.91	127.62	119.56
1	A	403	ALA	CA-C-N	-7.52	112.00	119.90
1	A	403	ALA	C-N-CA	-7.52	112.00	119.90
1	A	138	LYS	N-CA-C	7.34	119.32	110.07
1	D	99	TYR	CA-C-N	7.28	126.79	118.85
1	D	99	TYR	C-N-CA	7.28	126.79	118.85
1	C	77	ALA	O-C-N	7.00	131.33	122.23
1	A	15	ARG	CA-C-N	-6.98	117.56	122.59
1	A	15	ARG	C-N-CA	-6.98	117.56	122.59
1	B	267	PRO	N-CA-CB	6.77	110.36	103.25
1	C	5	ARG	N-CA-C	6.75	120.17	110.24
1	C	194	LEU	N-CA-C	6.52	118.94	111.11
1	B	345	VAL	CB-CA-C	-6.48	103.68	111.97
1	A	267	PRO	N-CA-CB	6.44	110.01	103.25
1	A	302	ARG	N-CA-C	-6.35	104.80	112.54
1	A	375	GLY	O-C-N	-6.32	117.34	123.35
1	A	386	ILE	N-CA-C	-6.24	103.50	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	VAL	N-CA-C	6.18	116.85	110.36
1	D	383	GLY	N-CA-C	-6.11	104.27	112.14
1	C	126	PHE	N-CA-C	-5.98	104.68	111.14
1	B	366	GLU	CA-C-N	5.89	127.20	119.84
1	B	366	GLU	C-N-CA	5.89	127.20	119.84
1	C	82	VAL	N-CA-C	5.86	115.41	108.96
1	C	272	THR	N-CA-C	5.72	118.46	111.82
1	D	300	CYS	N-CA-C	5.71	119.84	111.34
1	C	224	ALA	CA-C-N	-5.67	114.11	119.89
1	C	224	ALA	C-N-CA	-5.67	114.11	119.89
1	B	111	ILE	N-CA-C	5.57	118.13	108.95
1	D	360	LEU	CA-CB-CG	-5.43	97.29	116.30
1	B	300	CYS	CA-C-N	-5.40	114.98	122.86
1	B	300	CYS	C-N-CA	-5.40	114.98	122.86
1	A	224	ALA	CA-C-N	-5.37	114.25	119.78
1	A	224	ALA	C-N-CA	-5.37	114.25	119.78
1	C	8	THR	CB-CA-C	-5.34	103.05	110.37
1	D	301	GLY	N-CA-C	-5.29	100.64	113.18
1	D	380	ILE	CB-CA-C	5.29	117.97	111.25
1	D	196	GLU	N-CA-C	-5.28	105.48	112.34
1	B	301	GLY	N-CA-C	-5.22	108.48	114.69
1	A	354	ALA	N-CA-C	-5.21	102.81	110.52
1	C	77	ALA	CA-C-O	-5.18	114.49	120.24
1	C	405	LYS	N-CA-C	5.16	117.51	107.71
1	B	284	ALA	N-CA-C	-5.08	105.93	111.82
1	B	360	LEU	CA-CB-CG	-5.07	98.57	116.30
1	B	279	GLN	N-CA-C	5.04	116.46	111.07
1	D	299	GLY	CA-C-N	-5.00	115.60	121.90
1	D	299	GLY	C-N-CA	-5.00	115.60	121.90

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	85	0
1	B	3005	0	3073	80	0
1	C	2995	0	3076	102	0
1	D	3001	0	3070	96	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	354	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 (354) 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
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:HG2	1:C:271:ARG:NH1	1.86	0.86
1:A:309:GLN:HE21	1:A:309:GLN:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:235:MET:HG3	1:A:236:GLY:N	1.95	0.79
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:HG2	1:A:288:ARG:NH1	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:D:195:GLY:C	1:D:197:ASP:N	2.50	0.68
1:B:322:ARG:HH11	1:B:322:ARG:HG2	1.57	0.68
1:A:60:ASN:HD21	1:A:89:HIS:HB2	1.58	0.68
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:C:217:GLU:CD	1:C:220:ARG:HH12	2.03	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASP:O	1:D:40:THR:HG23	1.97	0.65
1:D:195:GLY:C	1:D:197:ASP:H	2.02	0.65
1:B:401:ARG:HA	1:B:401:ARG:CZ	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:A:160:ARG:C	1:A:160:ARG:HD2	2.23	0.64
1:C:41:THR:HG22	1:C:71:ILE:HG23	1.80	0.63
1:A:6:ARG:NH2	1:A:226:LEU:HG	2.14	0.63
1:C:159:ASP:OD1	1:D:302:ARG:NH1	2.31	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:B:96:LEU:HD12	1:B:103:ALA:HB2	1.81	0.62
1:D:62:GLU:HG2	1:D:95:LEU:CD2	2.29	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: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:HE21	1:A:309:GLN:CA	2.11	0.60
1:B:348:PRO:HD3	1:B:359:SER:OG	2.02	0.60
1:C:6:ARG:NH2	1:C:224:ALA:O	2.24	0.60
1:C:32:THR:HG21	1:C:39:ALA:O	2.00	0.60
1:C:91:ASN:C	1:C:91:ASN:ND2	2.59	0.60
1:C:24:ILE:HD13	1:C:251:LEU:HD22	1.83	0.60
1:D:62:GLU:HG2	1:D:95:LEU:HD21	1.84	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: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
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:A:97:ARG:HD3	1:A:128:GLU:OE2	2.04	0.58
1:D:32:THR:OG1	1:D:40:THR:HB	2.03	0.58
1:C:56:ARG:HD2	1:C:87:ASP:OD2	2.03	0.58
1:B:311:LEU:HD22	1:B:360:LEU:HD11	1.86	0.58
1:D:36:ASP:O	1:D:40:THR:HG22	2.04	0.58
1:D:111:ILE:HD11	1:D:142:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:N	1:A:355:HIS:HD2	1.92	0.57
1:B:96:LEU:HD23	1:B:129:MET:HE1	1.86	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:B:252:LEU:HD13	1:B:285:LEU:HD22	1.87	0.55
1:D:402:PHE:O	1:D:403:ALA:HB3	2.06	0.55
1:C:41:THR:HG21	1:C:74:ARG:HD2	1.86	0.55
1:D:403:ALA:HB1	1:D:404:PRO:CD	2.35	0.55
1:C:231:THR:O	1:C:232:GLU:HB3	2.06	0.55
1:A:171:HIS:NE2	1:A:210:ASP:OD2	2.39	0.55
1:D:113:PRO:HG2	1:D:144:ALA:HA	1.88	0.55
1:A:24:ILE:HD13	1:A:24:ILE:N	2.21	0.55
1:D:30:THR:HA	1:D:43:GLN:NE2	2.22	0.55
1:A:223:GLN:NE2	3:C:2018:HOH:O	2.41	0.54
1:B:258:THR:HG21	3:B:2010:HOH:O	2.07	0.54
1:C:326:TRP:HZ2	1:C:395:GLU:OE1	1.91	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:A:91:ASN:HD22	1:A:93:HIS:CE1	2.26	0.53
1:B:216:ARG:NH2	1:B:253:GLU:OE2	2.33	0.53
1:C:208:ALA:O	1:C:212:VAL:HG23	2.09	0.53
1:C:287:LEU:O	1:C:288:ARG:HG2	2.08	0.53
1:D:101:LYS:HD2	1:D:101:LYS:N	2.17	0.53
1:C:269:GLU:N	1:C:270:PRO:HD3	2.24	0.53
1:B:401:ARG:HA	1:B:401:ARG:NE	2.24	0.53
1:D:85:VAL:HG22	1:D:108:LYS:HB3	1.89	0.53
1:D:40:THR:O	1:D:44:VAL:HG12	2.09	0.53
1:B:9:PRO:HG3	1:B:196:GLU:HB3	1.90	0.53
1:C:265:PRO:HD3	1:C:271:ARG:HH12	1.74	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:A:238:LYS:NZ	3:A:2050:HOH:O	2.42	0.52
1:D:91:ASN:CB	3:D:2005:HOH:O	2.50	0.52
1:D:402:PHE:O	1:D:403:ALA:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:CD2	1:B:129:MET:HE1	2.38	0.52
1:B:337:LYS:H	1:B:355:HIS:CD2	2.28	0.52
1:C:231:THR:HB	1:C:232:GLU:OE1	2.09	0.52
1:C:373:ALA:C	1:C:374:ASP:OD1	2.52	0.52
1:A:238:LYS:NZ	1:A:238:LYS:HB2	2.24	0.51
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.10	0.51
1:B:90:PHE:CD1	1:B:90:PHE:N	2.68	0.51
1:C:217:GLU:OE2	1:C:220:ARG:NH1	2.38	0.51
1:A:311:LEU:HD23	1:A:360:LEU:HD11	1.92	0.51
1:C:128:GLU:O	1:C:132:ILE:HG13	2.11	0.51
1:D:215:TYR:CD2	1:D:228:LEU:HD23	2.45	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:A:389:GLU:HA	1:A:392:ARG:HH21	1.75	0.51
1:B:308:PHE:HA	1:B:360:LEU:HD13	1.92	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:C:381:LEU:O	1:C:383:GLY:N	2.40	0.50
1:D:279:GLN:NE2	1:D:288:ARG:HH21	2.05	0.50
1:C:57:LEU:HD21	1:C:84:LEU:HD23	1.94	0.50
1:D:161:ASN:HA	1:D:164:ARG:HD2	1.94	0.50
1:D:325:GLU:O	1:D:329:ARG:HB2	2.11	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:C:204:LYS:HE3	3:C:2012:HOH:O	2.11	0.49
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: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
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:A:395:GLU:O	1:A:399:LYS:HG3	2.12	0.49
1:B:390:PHE:O	1:B:394:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:N	1:C:270:PRO:CD	2.76	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:A:204:LYS:HE3	1:A:231:THR:HG21	1.95	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:223:GLN:NE2	3:C:2019:HOH:O	2.46	0.48
1:A:318:ARG:O	1:A:319:LEU:C	2.55	0.48
1:C:271:ARG:HH11	1:C:271:ARG:CG	2.00	0.48
1:C:81:GLU:O	1:C:81:GLU:HG3	2.13	0.48
1:D:90:PHE:CD1	1:D:90:PHE:C	2.91	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:31:ASN:C	1:D:31:ASN:HD22	2.22	0.48
1:C:285:LEU:O	1:D:209:ARG:NH1	2.47	0.48
1:C:389:GLU:O	1:C:393:LEU:HG	2.14	0.48
1:D:47:LEU:O	1:D:52:SER:HB3	2.14	0.48
1:C:356:ILE:HA	1:C:372:TYR:O	2.13	0.48
1:C:216:ARG:NH2	1:C:253:GLU:OE2	2.45	0.48
1:D:283:GLN:HG3	1:D:290:PHE:HD2	1.79	0.48
1:A:223:GLN:HE22	1:C:223:GLN:HE22	1.60	0.47
1:B:308:PHE:CZ	1:B:309:GLN:HG3	2.49	0.47
1:C:142:ILE:HD12	1:C:199:LEU:CD1	2.39	0.47
1:D:378:LEU:HG	1:D:379:THR:H	1.78	0.47
1:A:334:GLU:CD	1:A:334:GLU:H	2.22	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:385:GLY:O	1:D:386:ILE:C	2.57	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:O	1:A:376:LYS:HG3	2.05	0.47
1:C:37:VAL:HG13	1:C:71:ILE:HG13	1.96	0.47
1:D:142:ILE:CD1	1:D:199:LEU:HD11	2.45	0.46
1:D:382:LYS:HG2	1:D:386:ILE:CD1	2.45	0.46
1:C:150:ASP:HB3	1:C:153:LEU:CB	2.45	0.46
1:B:90:PHE:HD1	1:B:90:PHE:N	1.99	0.46
1:C:36:ASP:O	1:C:40:THR:HG22	2.15	0.46
1:D:331:PRO:HD2	1:D:403:ALA:CA	2.40	0.46
1:A:40:THR:O	1:A:44:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:HIS:HB3	1:B:90:PHE:HD1	1.79	0.46
1:C:91:ASN:C	1:C:91:ASN:HD22	2.23	0.46
1:D:381:LEU:C	1:D:383:GLY:N	2.72	0.46
1:C:237:VAL:O	1:C:238:LYS:C	2.59	0.46
1:A:220:ARG:NH1	1:C:187:GLU:OE2	2.42	0.46
1:A:45:LEU:O	1:A:49:ARG:HG3	2.16	0.46
1:C:31:ASN:N	1:C:43:GLN:OE1	2.48	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:C:205:VAL:HG12	1:C:206:SER:N	2.31	0.46
1:A:358:ILE:HB	1:A:390:PHE:CE1	2.51	0.46
1:B:392:ARG:HG3	1:B:392:ARG:HH11	1.81	0.46
1:C:78:GLU:C	1:C:80:VAL:H	2.24	0.45
1:C:318:ARG:O	1:C:322:ARG:HG2	2.16	0.45
1:A:238:LYS:HB2	1:A:238:LYS:HZ2	1.80	0.45
1:D:292:PRO:HD3	1:D:334:GLU:HA	1.98	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:D:394:VAL:O	1:D:398:VAL:HG23	2.16	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:C:373:ALA:C	1:C:374:ASP:CG	2.85	0.45
1:B:59:VAL:HG12	1:B:95:LEU:HD23	1.98	0.45
1:C:77:ALA:C	1:C:79:GLY:H	2.25	0.45
1:C:385:GLY:O	1:C:386:ILE:C	2.59	0.45
1:D:274:GLU:HA	1:D:277:VAL:HG13	1.98	0.45
1:C:74:ARG:O	1:C:78:GLU:N	2.45	0.44
1:B:209:ARG:HB2	3:B:2018:HOH:O	2.16	0.44
1:D:44:VAL:HB	1:D:55:VAL:HG11	1.99	0.44
1:D:177:ALA:O	1:D:181:SER:HB2	2.18	0.44
1:B:59:VAL:HB	1:B:88:PHE:CE1	2.53	0.44
1:B:392:ARG:HG3	1:B:392:ARG:NH1	2.33	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:C:360:LEU:O	1:C:361:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:PRO:O	1:B:272:THR:N	2.50	0.44
1:B:381:LEU:O	1:B:382:LYS:C	2.60	0.44
1:B:53:GLU:O	1:B:83:PRO:HD2	2.18	0.44
1:C:326:TRP:CZ2	1:C:395:GLU:OE1	2.71	0.44
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
1:D:35:ARG:HB3	1:D:63:GLU:HG3	1.99	0.43
1:B:24:ILE:HD12	1:B:287:LEU:HG	1.99	0.43
1:B:322:ARG:HG2	1:B:322:ARG:NH1	2.28	0.43
1:C:205:VAL:HG11	1:C:210:ASP:HB3	1.99	0.43
1:C:376:LYS:HB2	1:C:376:LYS:HE2	1.50	0.43
1:D:96:LEU:HD12	1:D:129:MET:HE2	1.99	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:C:370:PRO:HB3	1:C:376:LYS:HZ1	1.84	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:C:45:LEU:HD12	1:C:46:GLU:N	2.34	0.43
1:D:387:ALA:O	1:D:391:LEU:HB2	2.19	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:A:5:ARG:CZ	1:A:24:ILE:CD1	2.98	0.42
1:B:232:GLU:HA	1:B:262:SER:OG	2.20	0.42
1:B:231:THR:O	1:B:232:GLU:C	2.63	0.42
1:C:377:LEU:O	1:C:378:LEU:HB3	2.19	0.42
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.86	0.42
1:B:33:PRO:HB3	1:B:35:ARG:HH21	1.84	0.42
1:B:264:THR:HA	1:B:265:PRO:HD3	1.94	0.42
1:C:56:ARG:NE	1:C:141:ARG:HH22	2.18	0.42
1:A:149:LEU:HD23	1:A:149:LEU:HA	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:A:82:VAL:O	1:A:82:VAL:HG13	2.19	0.42
1:A:118:ARG:O	1:A:118:ARG:HG3	2.20	0.42
1:C:150:ASP:HB3	1:C:153:LEU:HB2	2.02	0.42
1:A:264:THR:HA	1:A:265:PRO:HD3	1.98	0.41
1:A:326:TRP:C	1:A:328:ALA:H	2.28	0.41
1:B:196:GLU:OE2	1:B:223:GLN:NE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:MET:HE1	1:C:273:LYS:HB3	2.02	0.41
1:A:26:VAL:HG12	1:A:27:GLN:N	2.35	0.41
1:A:316:SER:O	1:A:317:ARG:C	2.63	0.41
1:B:32:THR:OG1	1:B:40:THR:HB	2.20	0.41
1:B:318:ARG:HA	1:B:321:GLU:HG2	2.02	0.41
1:D:43:GLN:HA	1:D:46:GLU:HG2	2.02	0.41
1:D:383:GLY:C	1:D:385:GLY:N	2.78	0.41
1:C:24:ILE:HD12	1:C:287:LEU:HG	2.02	0.41
1:C:58:THR:HA	1:C:87:ASP:HB3	2.02	0.41
1:C:158:MET:HE2	1:C:173:VAL:HB	2.03	0.41
1:D:252:LEU:HA	1:D:252:LEU:HD23	1.87	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:A:327:ARG:HH11	1:A:327:ARG:HG3	1.85	0.41
1:B:37:VAL:HG22	1:B:67:ALA:HB1	2.02	0.41
1:C:56:ARG:CD	1:C:87:ASP:OD2	2.68	0.41
1:A:298:PRO:HB2	1:B:146:TRP:CH2	2.56	0.41
1:B:261:VAL:HG11	1:B:277:VAL:CG2	2.47	0.41
1:D:238:LYS:HE3	1:D:238:LYS:HB2	1.85	0.41
1:D:366:GLU:O	1:D:368:LYS:N	2.44	0.41
1:A:91:ASN:HA	1:A:93:HIS:CE1	2.55	0.41
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.88	0.41
1:A:209:ARG:HH11	1:A:209:ARG:HD2	1.69	0.41
1:B:60:ASN:HD21	1:B:89:HIS:CG	2.38	0.41
1:A:312:ALA:HB2	1:A:340:VAL:HB	2.02	0.41
1:B:38:GLU:HA	1:B:38:GLU:OE1	2.20	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:D:337:LYS:H	1:D:355:HIS:CD2	2.19	0.41
1:A:160:ARG:HD2	1:A:160:ARG:O	2.21	0.41
1:C:113:PRO:HG2	1:C:144:ALA:HA	2.03	0.41
1:D:138:LYS:HD3	1:D:138:LYS:HA	1.86	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:A:186:TYR:HB2	1:A:201:LEU:HD21	2.03	0.40
1:B:97:ARG:NH1	1:B:132:ILE:HG12	2.37	0.40
1:B:109:PHE:O	1:B:140:VAL:HA	2.21	0.40
1:C:44:VAL:HG22	1:C:55:VAL:HG11	2.02	0.40
1:D:61:ASP:CG	1:D:63:GLU:HB3	2.46	0.40
1:B:279:GLN:HB3	1:B:290:PHE:HZ	1.86	0.40
1:C:198:LYS:HD3	1:C:198:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:VAL:HA	1:D:83:PRO:HD2	1.93	0.40
1:A:187:GLU:OE1	1:C:220:ARG:NH2	2.53	0.40
1:B:260:ARG:NH2	1:B:274:GLU:OE2	2.45	0.40
1:C:90:PHE:O	1:C:91:ASN:CB	2.56	0.40
1:C:150:ASP:HA	1:C:151:PRO:HD2	1.96	0.40
1:C:234:GLY:C	1:C:236:GLY:H	2.29	0.40
1:D:131:ARG:O	1:D:134:MET:HG2	2.22	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%)	43 63
1	B	390/406 (96%)	367 (94%)	18 (5%)	5 (1%)	9 18
1	C	386/406 (95%)	348 (90%)	35 (9%)	3 (1%)	16 31
1	D	389/406 (96%)	351 (90%)	30 (8%)	8 (2%)	5 9
All	All	1566/1624 (96%)	1448 (92%)	101 (6%)	17 (1%)	11 22

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

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Mol	Chain	Res	Type
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%)	298 (93%)	22 (7%)	14	30
1	B	313/325 (96%)	274 (88%)	39 (12%)	4	9
1	C	313/325 (96%)	274 (88%)	39 (12%)	4	9
1	D	313/325 (96%)	261 (83%)	52 (17%)	2	4
All	All	1259/1300 (97%)	1107 (88%)	152 (12%)	5	10

All (152) 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	149	LEU
1	A	238	LYS
1	A	258	THR
1	A	260	ARG

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	288	ARG
1	A	309	GLN
1	A	323	LEU
1	A	334	GLU
1	A	376	LYS
1	A	382	LYS
1	A	384	GLU
1	A	386	ILE
1	A	392	ARG
1	B	18	ILE
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	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	230	LEU
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	277	VAL
1	B	287	LEU
1	B	306	THR
1	B	310	GLU
1	B	320	LYS
1	B	322	ARG
1	B	337	LYS

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Mol	Chain	Res	Type
1	B	345	VAL
1	B	374	ASP
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	37	VAL
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	104	GLU
1	C	113	PRO
1	C	115	THR
1	C	125	HIS
1	C	136	LEU
1	C	140	VAL
1	C	157	LEU
1	C	178	LEU
1	C	230	LEU
1	C	243	SER
1	C	247	LEU
1	C	252	LEU
1	C	258	THR
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

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Mol	Chain	Res	Type
1	C	336	LEU
1	C	374	ASP
1	C	376	LYS
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	70	GLU
1	D	72	LYS
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	129	MET
1	D	134	MET
1	D	140	VAL
1	D	166	GLU
1	D	181	SER
1	D	187	GLU
1	D	190	LEU
1	D	191	GLU
1	D	192	MET
1	D	194	LEU
1	D	198	LYS
1	D	204	LYS
1	D	216	ARG
1	D	218	LEU
1	D	230	LEU
1	D	232	GLU
1	D	260	ARG
1	D	277	VAL
1	D	283	GLN
1	D	288	ARG

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Mol	Chain	Res	Type
1	D	297	CYS
1	D	306	THR
1	D	310	GLU
1	D	315	VAL
1	D	316	SER
1	D	319	LEU
1	D	320	LYS
1	D	325	GLU
1	D	334	GLU
1	D	374	ASP
1	D	376	LYS
1	D	382	LYS
1	D	388	GLU
1	D	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	60	ASN
1	A	89	HIS
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
1	A	346	ASN
1	A	355	HIS
1	B	43	GLN
1	B	48	HIS
1	B	60	ASN
1	B	145	ASN
1	B	346	ASN
1	B	355	HIS
1	C	60	ASN
1	C	91	ASN
1	C	346	ASN
1	C	355	HIS
1	D	27	GLN
1	D	31	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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	B	501	1	0,12,12	-	-	-		
2	SF4	A	501	1	0,12,12	-	-	-		
2	SF4	D	501	1	0,12,12	-	-	-		
2	SF4	C	501	1	0,12,12	-	-	-		

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	B	501	1	-	-	0/6/5/5
2	SF4	A	501	1	-	-	0/6/5/5
2	SF4	D	501	1	-	-	0/6/5/5
2	SF4	C	501	1	-	-	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.51	2 (0%) 87 85	41, 69, 118, 151	0
1	B	394/406 (97%)	-0.40	4 (1%) 79 76	48, 79, 130, 164	0
1	C	392/406 (96%)	-0.22	3 (0%) 82 80	48, 87, 171, 206	0
1	D	393/406 (96%)	-0.21	3 (0%) 82 80	62, 93, 150, 243	0
All	All	1582/1624 (97%)	-0.34	12 (0%) 82 80	41, 82, 146, 243	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	ALA	4.4
1	A	375	GLY	4.3
1	D	404	PRO	2.6
1	B	286	GLY	2.5
1	D	406	ALA	2.5
1	A	381	LEU	2.4
1	B	375	GLY	2.3
1	B	114	GLY	2.3
1	C	233	ALA	2.2
1	D	405	LYS	2.2
1	C	406	ALA	2.1
1	B	382	LYS	2.1

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($\text{\AA}^2$)	Q<0.9
2	SF4	A	501	8/8	0.99	0.04	72,77,81,82	0
2	SF4	B	501	8/8	0.99	0.03	62,65,68,69	0
2	SF4	D	501	8/8	0.99	0.04	60,63,67,68	0
2	SF4	C	501	8/8	1.00	0.03	65,67,70,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.