



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 3PG9 / pdb_00003pg9
Title : Thermotoga maritima DAH7P synthase in complex with inhibitor
Authors : Cross, P.J.; Dobson, R.C.J.; Patchett, M.L.; Parker, E.J.
Deposited on : 2010-10-31
Resolution : 2.35 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)
Xtrriage (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

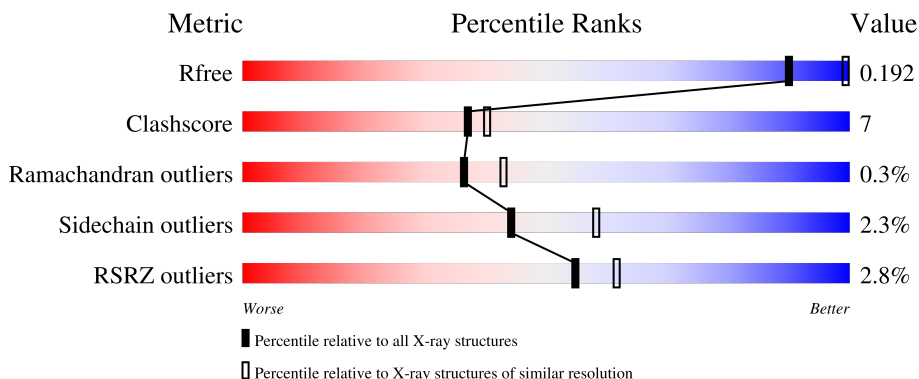
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	338	 3% 85% 14%
1	B	338	 0% 83% 16%
1	C	338	 4% 85% 15%
1	D	338	 3% 85% 14%
1	E	338	 2% 87% 13%

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Mol	Chain	Length	Quality of chain
1	F	338	 3% 83% 17%
1	G	338	 3% 82% 18%
1	H	338	 3% 84% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AZI	A	341	-	X	-	-
3	AZI	B	341	-	X	-	-
4	NO3	C	341	-	-	X	-
4	NO3	D	340	-	-	X	-
4	NO3	F	339	-	-	X	-

2 Entry composition

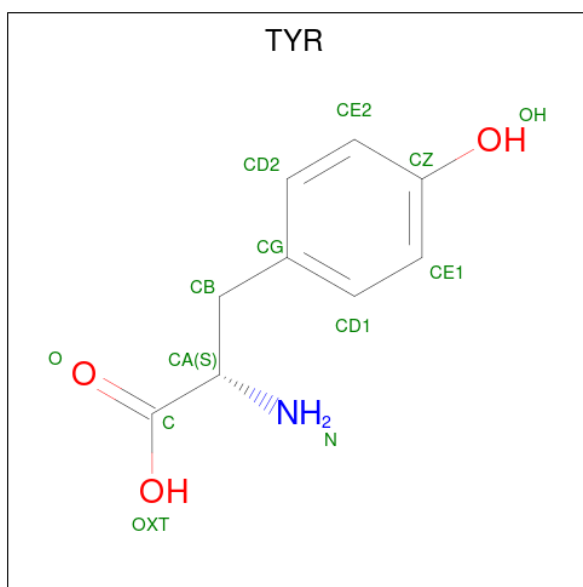
There are 6 unique types of molecules in this entry. The entry contains 21148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospho-2-dehydro-3-deoxyheptonate aldolase.

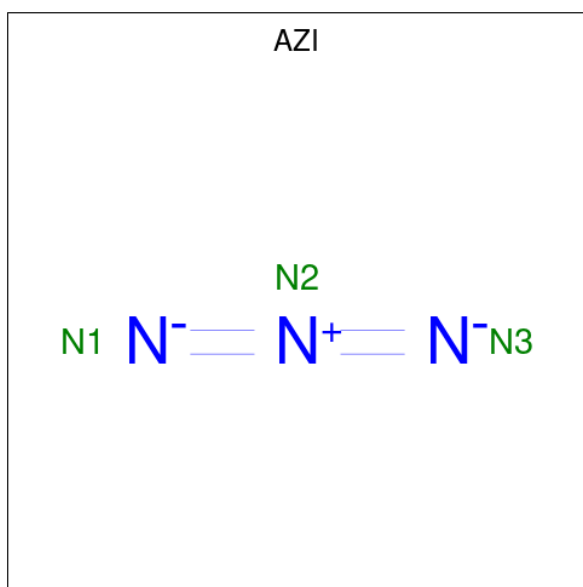
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2540	1627	424	479	10	0	0	0
1	B	338	2568	1641	431	486	10	0	0	0
1	C	338	2538	1623	429	476	10	0	1	0
1	D	338	2526	1613	421	482	10	0	0	0
1	E	338	2579	1643	436	490	10	0	0	0
1	F	338	2581	1643	439	489	10	0	0	0
1	G	338	2587	1652	434	491	10	0	1	0
1	H	338	2537	1622	431	474	10	0	0	0

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



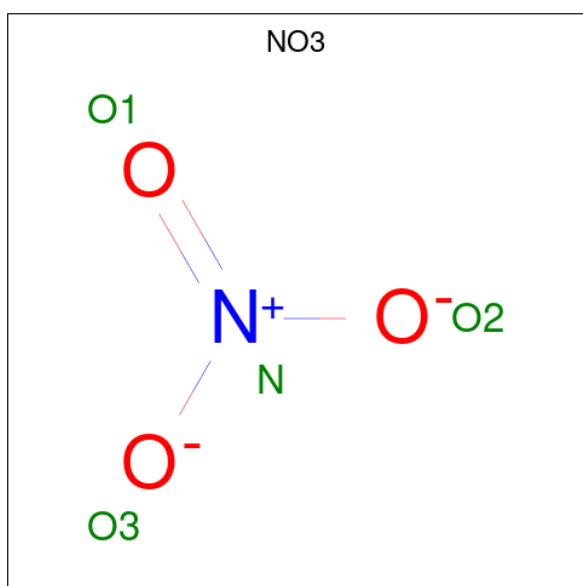
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	13	9	1	3	0	0
2	A	1	13	9	1	3	0	0
2	B	1	13	9	1	3	0	0
2	B	1	13	9	1	3	0	0
2	C	1	13	9	1	3	0	0
2	C	1	13	9	1	3	0	0
2	D	1	13	9	1	3	0	0
2	H	1	13	9	1	3	0	0

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 4 1 3	0	0
4	C	1	Total N O 4 1 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	N	O	0	0
			4	1	3		
4	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

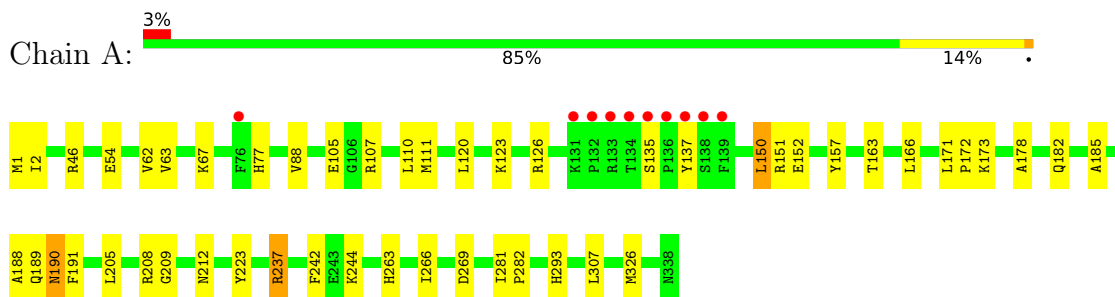
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total	O	0	0
			78	78		
6	B	81	Total	O	0	0
			81	81		
6	C	77	Total	O	0	0
			77	77		
6	D	61	Total	O	0	0
			61	61		
6	E	64	Total	O	0	0
			64	64		
6	F	65	Total	O	0	0
			65	65		
6	G	87	Total	O	0	0
			87	87		
6	H	52	Total	O	0	0
			52	52		

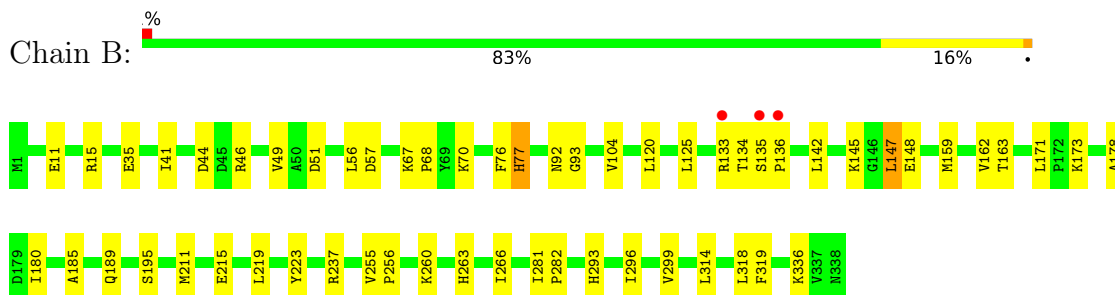
3 Residue-property plots [i](#)

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.

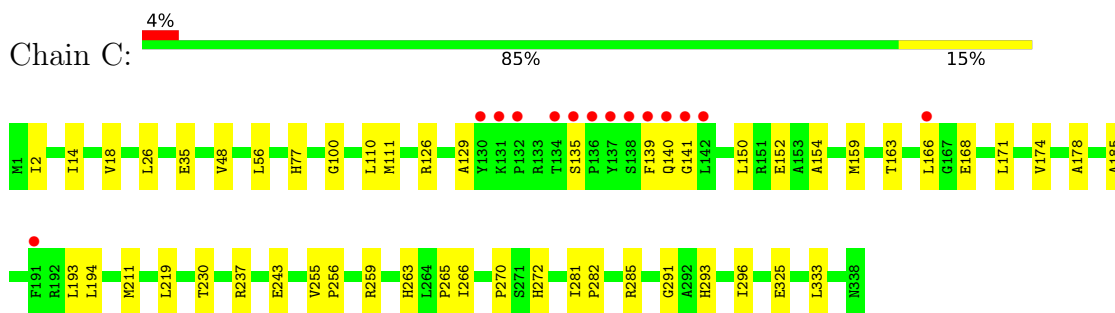
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



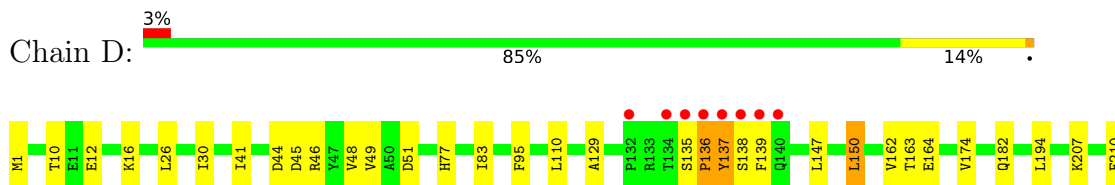
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

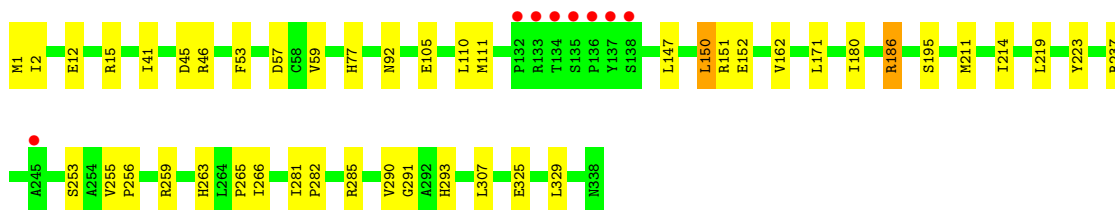
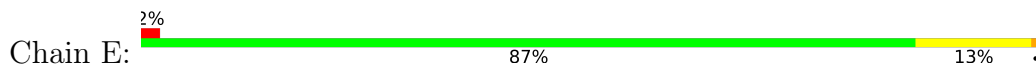


- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase

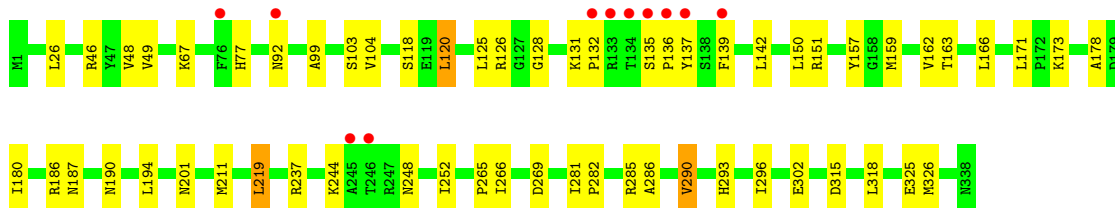
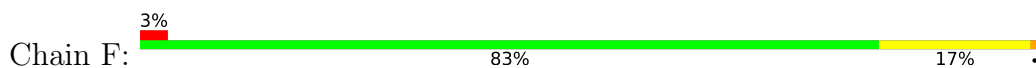




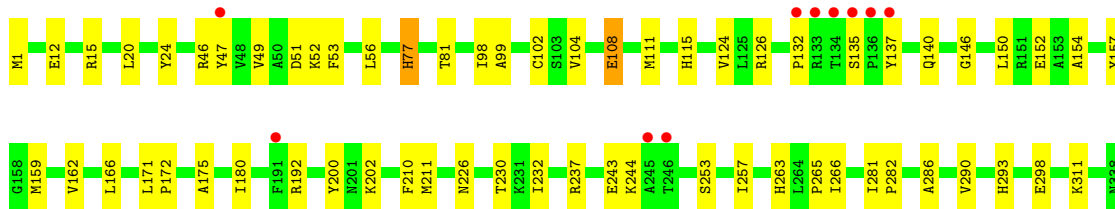
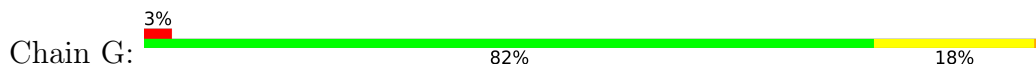
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



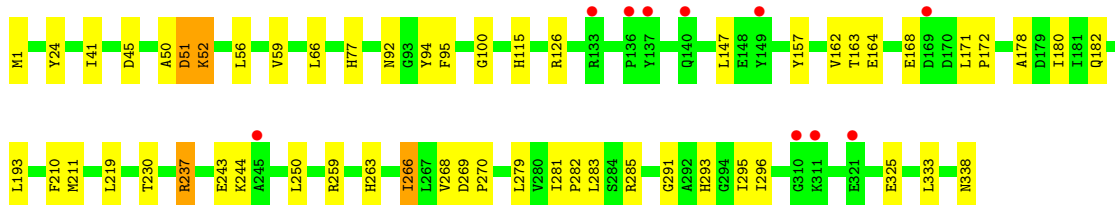
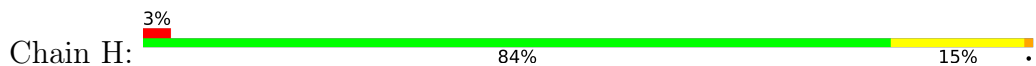
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 121.00Å 133.38Å 90.00° 92.12° 90.00°	Depositor
Resolution (Å)	52.57 – 2.35 52.57 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.2 (52.57-2.35) 97.2 (52.57-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.171 , 0.222 0.190 , 0.192	Depositor DCC
R_{free} test set	5203 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21148	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: CL, AZI, NO3

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	0.30	0/2582	0.69	0/3495
1	B	0.30	0/2611	0.70	2/3532 (0.1%)
1	C	0.30	0/2583	0.69	0/3496
1	D	0.29	0/2567	0.70	0/3481
1	E	0.29	0/2621	0.70	0/3543
1	F	0.29	0/2623	0.72	6/3543 (0.2%)
1	G	0.29	0/2630	0.71	2/3557 (0.1%)
1	H	0.29	0/2579	0.69	0/3492
All	All	0.29	0/20796	0.70	10/28139 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	77	HIS	CA-C-N	6.51	126.44	119.28
1	G	77	HIS	C-N-CA	6.51	126.44	119.28
1	F	302	GLU	CA-C-N	5.62	125.47	119.28
1	F	302	GLU	C-N-CA	5.62	125.47	119.28
1	F	77	HIS	CA-C-N	5.51	125.16	119.05
1	F	77	HIS	C-N-CA	5.51	125.16	119.05
1	B	77	HIS	CA-C-N	5.37	125.01	119.05
1	B	77	HIS	C-N-CA	5.37	125.01	119.05
1	F	269	ASP	CA-C-N	5.11	124.80	119.64
1	F	269	ASP	C-N-CA	5.11	124.80	119.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2525	33	0
1	B	2568	0	2572	38	0
1	C	2538	0	2517	34	0
1	D	2526	0	2469	30	0
1	E	2579	0	2587	36	0
1	F	2581	0	2603	43	0
1	G	2587	0	2583	42	0
1	H	2537	0	2530	49	0
2	A	26	0	16	0	0
2	B	26	0	16	0	0
2	C	26	0	16	0	0
2	D	13	0	8	1	0
2	H	13	0	8	0	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
4	A	4	0	0	1	0
4	C	4	0	0	2	0
4	D	4	0	0	2	0
4	F	4	0	0	2	0
5	B	1	0	0	0	0
6	A	78	0	0	1	0
6	B	81	0	0	0	0
6	C	77	0	0	0	0
6	D	61	0	0	1	0
6	E	64	0	0	2	0
6	F	65	0	0	2	0
6	G	87	0	0	1	0
6	H	52	0	0	2	0
All	All	21148	0	20450	291	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 7.

All (291) 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:B:68:PRO:HG2	1:B:219:LEU:HD11	1.43	1.01
1:F:266:ILE:H	1:F:293:HIS:HD2	1.05	1.00
1:H:164:GLU:HB2	1:H:182:GLN:HE21	1.27	0.98
1:C:266:ILE:H	1:C:293:HIS:HD2	1.11	0.97
1:F:290:VAL:HG13	1:G:286:ALA:HB2	1.49	0.93
1:B:92:ASN:ND2	1:B:93:GLY:H	1.69	0.90
1:H:266:ILE:H	1:H:293:HIS:HD2	1.17	0.90
1:G:104:VAL:HG21	1:G:150:LEU:HD21	1.60	0.83
1:G:162:VAL:HG22	1:G:180:ILE:HB	1.58	0.83
1:E:266:ILE:H	1:E:293:HIS:HD2	1.30	0.79
1:D:266:ILE:H	1:D:293:HIS:HD2	1.28	0.79
1:B:266:ILE:H	1:B:293:HIS:HD2	1.31	0.79
1:H:162:VAL:HG22	1:H:180:ILE:HB	1.65	0.77
1:A:237:ARG:O	1:A:237:ARG:HG2	1.86	0.75
1:B:49:VAL:HG12	1:B:51:ASP:H	1.52	0.75
1:A:266:ILE:H	1:A:293:HIS:HD2	1.35	0.74
1:F:132:PRO:HG3	1:F:186:ARG:HH21	1.53	0.74
1:H:266:ILE:H	1:H:293:HIS:CD2	2.03	0.74
1:H:52:LYS:H	1:H:52:LYS:NZ	1.86	0.73
1:G:108:GLU:CD	1:G:108:GLU:H	1.95	0.73
1:B:92:ASN:CG	1:B:93:GLY:H	1.97	0.73
4:D:340:NO3:O2	1:E:211:MET:HA	1.90	0.71
1:F:266:ILE:H	1:F:293:HIS:CD2	1.98	0.70
1:F:166:LEU:HD11	1:F:186:ARG:NH2	2.06	0.70
1:B:237:ARG:HG2	1:B:237:ARG:O	1.93	0.68
1:B:134:THR:HG23	1:B:135:SER:H	1.59	0.68
1:C:266:ILE:H	1:C:293:HIS:CD2	2.03	0.68
1:G:266:ILE:H	1:G:293:HIS:HD2	1.41	0.68
1:H:24:TYR:OH	1:H:52:LYS:HE3	1.95	0.67
1:D:266:ILE:H	1:D:293:HIS:CD2	2.10	0.67
1:C:168:GLU:HA	1:C:171:LEU:HD23	1.79	0.65
1:E:186:ARG:CD	1:E:186:ARG:H	2.10	0.65
1:E:15:ARG:HD3	6:E:342:HOH:O	1.96	0.64
1:D:49:VAL:HG22	1:D:51:ASP:H	1.61	0.64
1:E:186:ARG:H	1:E:186:ARG:HD2	1.63	0.64
1:G:210:PHE:HB3	1:G:237:ARG:HH21	1.61	0.64
1:D:1:MET:HB2	1:D:45:ASP:OD2	1.98	0.63
1:F:162:VAL:HG22	1:F:180:ILE:HB	1.80	0.63
1:F:286:ALA:O	1:F:290:VAL:HG22	1.99	0.63
1:H:171:LEU:HD21	1:H:193:LEU:HD11	1.81	0.63
1:C:237:ARG:HE	1:C:272[B]:HIS:CD2	2.16	0.62
1:A:77:HIS:HB3	1:A:263:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:MET:HE2	1:F:326:MET:HA	1.82	0.62
1:G:77:HIS:HB3	1:G:263:HIS:CD2	2.35	0.62
1:C:77:HIS:HB3	1:C:263:HIS:CD2	2.34	0.62
1:F:103:SER:HG	1:F:139:PHE:HE2	1.48	0.62
1:F:266:ILE:N	1:F:293:HIS:HD2	1.88	0.62
1:G:104:VAL:HG21	1:G:150:LEU:CD2	2.27	0.61
1:D:10:THR:OG1	1:D:12:GLU:HG2	2.00	0.61
1:G:49:VAL:HG12	1:G:51:ASP:H	1.65	0.61
1:E:1:MET:HE1	1:E:53:PHE:CD2	2.36	0.61
1:C:211:MET:HA	4:C:341:NO3:O1	2.01	0.60
1:A:182:GLN:HE21	1:A:205:LEU:HD23	1.65	0.60
1:E:77:HIS:HB3	1:E:263:HIS:CD2	2.36	0.60
1:A:46:ARG:HG3	1:A:67:LYS:O	2.01	0.60
1:G:98:ILE:HG23	1:G:124:VAL:HG12	1.84	0.59
1:B:92:ASN:CG	1:B:93:GLY:N	2.60	0.59
1:H:168:GLU:HA	1:H:171:LEU:HD23	1.85	0.59
1:C:237:ARG:HH21	1:C:272[B]:HIS:CD2	2.22	0.58
1:A:1:MET:HE3	1:A:62:VAL:HG11	1.86	0.58
1:F:128:GLY:HA3	1:F:131:LYS:HE3	1.86	0.58
1:C:230:THR:O	1:C:230:THR:HG22	2.04	0.58
1:F:237:ARG:O	1:F:237:ARG:HG2	2.02	0.58
1:E:12:GLU:HG2	1:E:15:ARG:NH2	2.19	0.57
1:B:215:GLU:O	1:B:219:LEU:HD13	2.04	0.57
1:G:52:LYS:HB2	6:G:577:HOH:O	2.04	0.57
1:F:126:ARG:HD2	1:F:296:ILE:HG13	1.87	0.56
1:B:211:MET:HA	4:F:339:NO3:O1	2.05	0.56
1:E:255:VAL:HB	1:E:256:PRO:HD3	1.87	0.56
1:B:266:ILE:H	1:B:293:HIS:CD2	2.19	0.56
1:G:1:MET:HE1	1:G:53:PHE:CD2	2.40	0.56
1:A:266:ILE:H	1:A:293:HIS:CD2	2.21	0.56
1:A:54:GLU:HB3	1:G:311:LYS:HD2	1.88	0.56
1:C:154:ALA:HB1	1:C:159:MET:O	2.06	0.55
1:G:111:MET:HE1	1:G:152:GLU:HG2	1.88	0.55
1:D:110:LEU:HD21	1:D:150:LEU:HD13	1.89	0.55
1:A:191:PHE:HD1	1:A:223:TYR:CG	2.25	0.55
1:B:11:GLU:O	1:B:15:ARG:HG3	2.07	0.55
1:F:211:MET:HA	4:F:339:NO3:O3	2.08	0.54
1:H:95:PHE:CZ	1:H:295:ILE:HG23	2.43	0.54
1:D:12:GLU:O	1:D:16:LYS:HG3	2.08	0.54
1:D:210:PHE:HB3	1:D:237:ARG:HH21	1.73	0.54
1:E:285:ARG:HD3	1:E:325:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ILE:HB	1:F:282:PRO:HD3	1.90	0.54
1:H:52:LYS:H	1:H:52:LYS:HZ2	1.52	0.53
1:G:24:TYR:OH	1:G:52:LYS:HE3	2.09	0.53
1:H:1:MET:HB2	1:H:45:ASP:OD2	2.09	0.53
1:G:266:ILE:H	1:G:293:HIS:CD2	2.24	0.53
1:A:189:GLN:O	1:A:190:ASN:HB3	2.09	0.53
1:D:77:HIS:HB3	1:D:263:HIS:CD2	2.44	0.52
1:A:105:GLU:HB3	1:A:307:LEU:HD22	1.91	0.52
1:F:285:ARG:HA	1:F:326:MET:HE1	1.92	0.52
1:D:164:GLU:HB2	1:D:182:GLN:HE21	1.75	0.52
1:A:137:TYR:CB	1:G:47:TYR:HB3	2.40	0.51
1:C:265:PRO:HA	1:C:293:HIS:CD2	2.45	0.51
1:C:35:GLU:OE2	1:E:46:ARG:NH2	2.43	0.51
1:D:95:PHE:HA	1:D:293:HIS:O	2.11	0.51
1:G:243:GLU:C	1:G:244:LYS:HE2	2.36	0.51
1:D:285:ARG:HA	1:D:326:MET:HE1	1.92	0.51
1:H:259:ARG:HD2	1:H:291:GLY:O	2.11	0.51
1:E:266:ILE:H	1:E:293:HIS:CD2	2.20	0.51
1:H:94:TYR:HB3	1:H:338:ASN:HD21	1.75	0.51
1:B:163:THR:HG22	1:B:178:ALA:HB2	1.91	0.51
1:E:1:MET:HB2	1:E:45:ASP:OD2	2.11	0.51
1:B:68:PRO:CG	1:B:219:LEU:HD11	2.29	0.50
1:C:259:ARG:HD2	1:C:291:GLY:O	2.12	0.50
1:F:285:ARG:HD3	1:F:325:GLU:OE1	2.12	0.50
1:G:132:PRO:HA	1:G:166:LEU:HD21	1.92	0.50
1:F:166:LEU:HD11	1:F:186:ARG:HH22	1.77	0.50
1:G:99:ALA:C	1:G:126:ARG:HG2	2.37	0.50
1:F:92:ASN:OD1	1:F:293:HIS:HE1	1.95	0.49
1:F:187:ASN:ND2	1:F:190:ASN:HD22	2.10	0.49
1:G:108:GLU:CD	1:G:108:GLU:N	2.69	0.49
1:B:134:THR:HG23	1:B:135:SER:N	2.27	0.49
1:B:211:MET:HE2	1:F:211:MET:HE2	1.94	0.49
1:D:129:ALA:HA	6:D:367:HOH:O	2.11	0.49
1:G:281:ILE:HB	1:G:282:PRO:HD3	1.94	0.49
1:H:92:ASN:OD1	1:H:293:HIS:HE1	1.96	0.49
1:H:24:TYR:CE2	1:H:52:LYS:HE3	2.48	0.49
1:A:166:LEU:HD23	1:G:192:ARG:NH2	2.28	0.49
1:D:135:SER:O	1:D:137:TYR:N	2.46	0.49
1:H:171:LEU:HD21	1:H:193:LEU:CD1	2.42	0.49
1:C:26:LEU:HD11	1:C:48:VAL:HG21	1.94	0.48
1:E:329:LEU:HD21	1:H:333:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:GLU:O	1:G:244:LYS:HE2	2.13	0.48
1:A:107:ARG:O	1:A:111:MET:HG2	2.13	0.48
1:B:104:VAL:HG12	1:B:142:LEU:HD12	1.95	0.48
1:F:49:VAL:HG22	6:F:344:HOH:O	2.13	0.48
1:E:110:LEU:HD21	1:E:150:LEU:HA	1.95	0.48
1:C:110:LEU:HD21	1:C:150:LEU:HD23	1.95	0.48
1:F:151:ARG:O	1:F:151:ARG:HD3	2.13	0.48
1:H:163:THR:HG22	1:H:178:ALA:HB2	1.95	0.48
1:B:41:ILE:N	1:B:41:ILE:HD12	2.28	0.48
1:F:103:SER:OG	1:F:139:PHE:HE2	1.95	0.48
1:C:185:ALA:HB2	1:C:237:ARG:HD3	1.95	0.48
1:A:326:MET:HE2	1:A:326:MET:HA	1.95	0.48
1:H:270:PRO:HD2	1:H:296:ILE:O	2.14	0.48
1:C:163:THR:HG22	1:C:178:ALA:HB2	1.96	0.47
1:G:146:GLY:O	1:G:150:LEU:HD23	2.13	0.47
1:A:188:ALA:HB1	1:A:212:ASN:OD1	2.14	0.47
1:G:135:SER:C	1:G:137:TYR:H	2.22	0.47
1:H:250:LEU:HD23	1:H:283:LEU:HD22	1.97	0.47
1:F:265:PRO:HA	1:F:293:HIS:CD2	2.50	0.47
1:E:265:PRO:HA	1:E:293:HIS:CD2	2.50	0.47
1:A:111:MET:HE3	1:A:157:TYR:HE2	1.80	0.47
1:F:92:ASN:CG	1:F:293:HIS:HE1	2.22	0.47
1:A:110:LEU:HD21	1:A:150:LEU:HD13	1.97	0.47
1:G:154:ALA:HB1	1:G:159:MET:O	2.15	0.47
1:E:256:PRO:HG3	1:E:290:VAL:HG22	1.96	0.47
1:F:99:ALA:C	1:F:126:ARG:HG2	2.40	0.47
1:C:2:ILE:HG21	1:E:2:ILE:CD1	2.45	0.46
1:F:315:ASP:OD1	1:F:318:LEU:HD23	2.15	0.46
1:B:314:LEU:HD22	1:B:318:LEU:HB3	1.96	0.46
1:C:163:THR:HG23	1:C:174:VAL:HG13	1.97	0.46
1:C:266:ILE:N	1:C:293:HIS:HD2	1.95	0.46
1:E:12:GLU:HG2	1:E:15:ARG:HH21	1.80	0.46
1:H:115:HIS:HB2	1:H:157:TYR:CZ	2.50	0.46
1:B:145:LYS:HD3	1:B:148:GLU:OE2	2.15	0.46
1:D:30:ILE:HD12	1:D:30:ILE:N	2.30	0.46
1:D:285:ARG:HD3	1:D:325:GLU:OE2	2.15	0.46
1:A:107:ARG:HH21	1:A:152:GLU:CD	2.23	0.46
1:A:151:ARG:O	1:A:151:ARG:HD3	2.16	0.46
1:A:171:LEU:HB3	1:A:172:PRO:HD3	1.98	0.46
1:C:14:ILE:O	1:C:18:VAL:HG23	2.16	0.46
1:H:115:HIS:CD2	1:H:157:TYR:CE1	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:LYS:HA	1:H:244:LYS:HD3	1.76	0.46
1:C:281:ILE:HB	1:C:282:PRO:HD3	1.97	0.46
1:F:135:SER:HB2	1:F:136:PRO:HD2	1.98	0.46
1:G:210:PHE:HB3	1:G:237:ARG:NH2	2.31	0.46
1:C:111:MET:HE1	1:C:152:GLU:HG2	1.98	0.45
1:E:41:ILE:N	1:E:41:ILE:HD12	2.31	0.45
1:F:163:THR:HG22	1:F:178:ALA:HB2	1.98	0.45
1:G:232:ILE:O	1:G:265:PRO:HD2	2.16	0.45
1:A:189:GLN:O	1:A:190:ASN:CB	2.64	0.45
1:E:151:ARG:O	1:E:151:ARG:HD3	2.17	0.45
1:G:102:CYS:HB2	1:G:298:GLU:OE2	2.16	0.45
1:H:52:LYS:HB2	1:H:52:LYS:HE2	1.49	0.45
1:D:44:ASP:OD2	1:D:46:ARG:HB2	2.16	0.45
1:E:259:ARG:HD2	1:E:291:GLY:O	2.16	0.45
1:H:279:LEU:C	1:H:282:PRO:HD2	2.41	0.45
1:G:237:ARG:HG2	1:G:237:ARG:O	2.17	0.45
1:H:52:LYS:H	1:H:52:LYS:HZ3	1.62	0.45
1:A:185:ALA:HB1	1:A:209:GLY:HA2	1.99	0.45
1:B:125:LEU:HB2	1:B:159:MET:HE2	1.99	0.45
1:H:77:HIS:HB3	1:H:263:HIS:CD2	2.51	0.45
1:H:237:ARG:HB3	1:H:269:ASP:HB3	1.98	0.45
1:H:266:ILE:N	1:H:293:HIS:HD2	1.99	0.45
1:G:230:THR:HG22	1:G:230:THR:O	2.16	0.45
1:H:210:PHE:HB3	1:H:237:ARG:NH1	2.31	0.45
1:E:259:ARG:HA	6:E:368:HOH:O	2.17	0.44
1:F:92:ASN:OD1	1:F:293:HIS:CE1	2.70	0.44
1:E:111:MET:HE1	1:E:152:GLU:HG2	1.99	0.44
1:H:230:THR:HG22	6:H:536:HOH:O	2.17	0.44
1:B:46:ARG:HG3	1:B:67:LYS:O	2.18	0.44
1:E:253:SER:HB3	1:H:283:LEU:HD21	1.99	0.44
1:F:104:VAL:HG12	1:F:142:LEU:HD12	1.98	0.44
1:G:115:HIS:HB2	1:G:157:TYR:CZ	2.53	0.44
1:B:76:PHE:HB2	3:B:341:AZI:N3	2.33	0.44
1:D:135:SER:O	1:D:136:PRO:C	2.61	0.44
1:H:24:TYR:CZ	1:H:52:LYS:HE3	2.52	0.44
1:C:129:ALA:O	1:C:141:GLY:HA3	2.18	0.44
1:F:237:ARG:HH12	1:F:248:ASN:CG	2.26	0.44
1:E:186:ARG:HD2	1:E:186:ARG:N	2.31	0.44
1:C:285:ARG:HD3	1:C:325:GLU:OE2	2.17	0.43
1:F:252:ILE:HD11	1:F:290:VAL:HG21	2.00	0.43
1:C:139:PHE:HD1	1:C:140:GLN:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ILE:HG13	1:H:243:GLU:OE1	2.18	0.43
1:A:242:PHE:O	1:A:244:LYS:HE2	2.18	0.43
1:G:20:LEU:HD21	1:G:52:LYS:HB3	1.99	0.43
1:H:164:GLU:HB2	1:H:182:GLN:NE2	2.11	0.43
1:D:83:ILE:HD12	1:D:233:ILE:HG13	2.00	0.43
1:G:175:ALA:O	1:G:202:LYS:HE3	2.19	0.43
1:A:88:VAL:HG21	1:A:123:LYS:HB3	1.99	0.43
1:B:281:ILE:HB	1:B:282:PRO:HD3	2.00	0.43
1:E:162:VAL:HG22	1:E:180:ILE:HB	2.01	0.43
1:B:46:ARG:HD2	1:B:70:LYS:HB2	2.01	0.43
1:H:50:ALA:O	1:H:51:ASP:C	2.62	0.43
1:H:269:ASP:OD1	1:H:269:ASP:C	2.62	0.43
1:B:35:GLU:OE2	1:G:46:ARG:NH2	2.51	0.43
1:E:105:GLU:HG2	1:E:307:LEU:HD22	2.01	0.43
1:G:171:LEU:HB3	1:G:172:PRO:HD3	2.01	0.43
1:C:126:ARG:HD3	1:C:126:ARG:C	2.44	0.42
1:C:255:VAL:HB	1:C:256:PRO:CD	2.49	0.42
1:A:2:ILE:HB	1:A:63:VAL:HB	2.02	0.42
1:A:208:ARG:HD3	6:A:360:HOH:O	2.18	0.42
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.82	0.42
4:C:341:NO3:O3	1:H:211:MET:HA	2.20	0.42
1:B:147:LEU:HD23	1:B:173:LYS:HB3	2.01	0.42
1:C:270:PRO:HD2	1:C:296:ILE:O	2.20	0.42
1:D:211:MET:HA	4:D:340:NO3:O3	2.19	0.42
1:E:281:ILE:HB	1:E:282:PRO:HD3	2.01	0.42
1:H:171:LEU:HB2	1:H:172:PRO:HD3	2.01	0.42
1:H:285:ARG:HD3	1:H:325:GLU:OE2	2.19	0.42
1:A:237:ARG:HB2	1:A:269:ASP:HB3	1.99	0.42
1:B:185:ALA:HB2	1:B:237:ARG:HD2	2.00	0.42
1:C:243:GLU:OE2	1:D:214:ILE:N	2.49	0.42
1:F:118:SER:OG	1:F:157:TYR:HB3	2.19	0.42
1:F:135:SER:C	1:F:137:TYR:H	2.27	0.42
1:A:281:ILE:HB	1:A:282:PRO:HD3	2.01	0.42
1:B:77:HIS:HB3	1:B:263:HIS:CD2	2.55	0.42
1:C:333:LEU:HD21	1:D:329:LEU:HD21	2.02	0.42
1:F:120:LEU:HD12	1:F:120:LEU:HA	1.87	0.42
1:E:1:MET:HE1	1:E:53:PHE:CG	2.55	0.42
1:H:100:GLY:HA3	1:H:126:ARG:HG2	2.00	0.42
1:D:304:GLU:OE2	1:E:57:ASP:HB2	2.20	0.42
1:E:255:VAL:O	1:E:259:ARG:HG3	2.20	0.42
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HD22	1:D:224:ILE:HD11	2.02	0.41
1:B:135:SER:HB2	1:B:136:PRO:HD2	2.02	0.41
1:B:173:LYS:HA	1:B:173:LYS:HD3	1.86	0.41
1:B:299:VAL:HG21	1:B:319:PHE:CD1	2.56	0.41
1:D:26:LEU:HD11	1:D:48:VAL:HG21	2.02	0.41
1:H:115:HIS:CD2	1:H:157:TYR:HE1	2.38	0.41
1:F:219:LEU:HD12	1:F:219:LEU:HA	1.80	0.41
1:H:1:MET:HE3	1:H:41:ILE:HG12	2.02	0.41
1:H:115:HIS:HD2	1:H:157:TYR:CE1	2.38	0.41
1:A:1:MET:HE3	1:A:62:VAL:CG1	2.50	0.41
1:A:163:THR:HG22	1:A:178:ALA:HB2	2.03	0.41
1:D:163:THR:HG23	1:D:174:VAL:HG13	2.01	0.41
1:E:150:LEU:HA	1:E:150:LEU:HD12	1.94	0.41
1:F:126:ARG:HA	1:F:162:VAL:O	2.20	0.41
1:F:125:LEU:HB2	1:F:159:MET:HE2	2.02	0.41
1:H:1:MET:N	6:H:416:HOH:O	2.50	0.41
4:A:342:NO3:O2	1:G:211:MET:HA	2.21	0.41
1:B:44:ASP:OD2	1:B:46:ARG:HB2	2.20	0.41
1:C:166:LEU:HD12	1:C:166:LEU:HA	1.96	0.41
1:C:255:VAL:HB	1:C:256:PRO:HD3	2.03	0.41
1:E:195:SER:HB3	1:E:223:TYR:HE1	1.86	0.41
1:H:281:ILE:HB	1:H:282:PRO:HD3	2.02	0.41
1:A:173:LYS:HA	1:A:173:LYS:HD3	1.92	0.41
1:D:138:SER:O	1:D:139:PHE:C	2.64	0.41
1:F:26:LEU:HD11	1:F:48:VAL:HG21	2.01	0.41
1:G:171:LEU:HG	1:G:200:TYR:CE2	2.55	0.41
1:B:162:VAL:HG22	1:B:180:ILE:HB	2.02	0.41
1:B:195:SER:HB3	1:B:223:TYR:HE1	1.86	0.41
1:H:100:GLY:CA	1:H:126:ARG:HG2	2.51	0.41
1:B:255:VAL:HB	1:B:256:PRO:CD	2.51	0.41
1:D:315:ASP:OD1	1:D:318:LEU:HB2	2.21	0.41
2:D:339:TYR:HA	1:H:66:LEU:HD11	2.03	0.41
1:C:100:GLY:HA3	1:C:126:ARG:O	2.21	0.40
1:D:150:LEU:HD12	1:D:150:LEU:HA	1.89	0.40
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.89	0.40
1:B:256:PRO:O	1:B:260:LYS:HD3	2.22	0.40
1:F:46:ARG:HG2	1:F:67:LYS:O	2.21	0.40
1:F:173:LYS:HD3	1:F:173:LYS:HA	1.91	0.40
6:F:375:HOH:O	1:G:243:GLU:HG2	2.21	0.40
1:H:56:LEU:HB2	1:H:59:VAL:HG23	2.03	0.40
1:G:253:SER:O	1:G:257:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HE3	1:D:41:ILE:HG13	2.02	0.40
1:E:53:PHE:O	1:E:59:VAL:HG21	2.22	0.40
1:G:12:GLU:O	1:G:15:ARG:HB2	2.21	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	336/338 (99%)	324 (96%)	10 (3%)	2 (1%)	21	24
1	B	336/338 (99%)	329 (98%)	6 (2%)	1 (0%)	36	43
1	C	337/338 (100%)	329 (98%)	7 (2%)	1 (0%)	36	43
1	D	336/338 (99%)	325 (97%)	9 (3%)	2 (1%)	21	24
1	E	336/338 (99%)	328 (98%)	8 (2%)	0	100	100
1	F	336/338 (99%)	328 (98%)	8 (2%)	0	100	100
1	G	337/338 (100%)	328 (97%)	9 (3%)	0	100	100
1	H	336/338 (99%)	328 (98%)	7 (2%)	1 (0%)	36	43
All	All	2690/2704 (100%)	2619 (97%)	64 (2%)	7 (0%)	36	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	136	PRO
1	D	137	TYR
1	A	190	ASN
1	C	135	SER
1	H	51	ASP
1	A	135	SER
1	B	133	ARG

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	259/286 (91%)	255 (98%)	4 (2%)	57 72
1	B	268/286 (94%)	260 (97%)	8 (3%)	36 48
1	C	258/286 (90%)	255 (99%)	3 (1%)	63 77
1	D	254/286 (89%)	247 (97%)	7 (3%)	38 51
1	E	271/286 (95%)	264 (97%)	7 (3%)	40 54
1	F	273/286 (96%)	265 (97%)	8 (3%)	37 49
1	G	269/286 (94%)	263 (98%)	6 (2%)	45 59
1	H	260/286 (91%)	254 (98%)	6 (2%)	44 58
All	All	2112/2288 (92%)	2063 (98%)	49 (2%)	44 58

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LEU
1	A	126	ARG
1	A	150	LEU
1	A	237	ARG
1	B	56	LEU
1	B	57	ASP
1	B	120	LEU
1	B	147	LEU
1	B	171	LEU
1	B	189	GLN
1	B	296	ILE
1	B	336	LYS
1	C	56	LEU
1	C	193	LEU
1	C	194	LEU
1	D	147	LEU
1	D	150	LEU
1	D	162	VAL
1	D	207	LYS

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Mol	Chain	Res	Type
1	D	219	LEU
1	D	290	VAL
1	D	318	LEU
1	E	92	ASN
1	E	147	LEU
1	E	150	LEU
1	E	171	LEU
1	E	186	ARG
1	E	219	LEU
1	E	237	ARG
1	F	120	LEU
1	F	150	LEU
1	F	171	LEU
1	F	194	LEU
1	F	201	ASN
1	F	219	LEU
1	F	244	LYS
1	F	290	VAL
1	G	56	LEU
1	G	81	THR
1	G	108	GLU
1	G	140	GLN
1	G	226	ASN
1	G	290	VAL
1	H	52	LYS
1	H	147	LEU
1	H	219	LEU
1	H	237	ARG
1	H	266	ILE
1	H	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	248	ASN
1	A	293	HIS
1	B	92	ASN
1	B	187	ASN
1	B	189	GLN
1	B	212	ASN
1	B	293	HIS

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Mol	Chain	Res	Type
1	B	324	GLN
1	C	115	HIS
1	C	189	GLN
1	C	212	ASN
1	C	293	HIS
1	D	182	GLN
1	D	187	ASN
1	D	189	GLN
1	D	212	ASN
1	D	293	HIS
1	D	312	GLN
1	E	182	GLN
1	E	187	ASN
1	E	212	ASN
1	E	272	HIS
1	E	293	HIS
1	F	115	HIS
1	F	187	ASN
1	F	293	HIS
1	G	187	ASN
1	G	212	ASN
1	G	293	HIS
1	H	115	HIS
1	H	182	GLN
1	H	187	ASN
1	H	293	HIS
1	H	338	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NO3	C	341	-	1,3,3	3.17	1 (100%)	0,3,3	-	-
4	NO3	D	340	-	1,3,3	3.22	1 (100%)	0,3,3	-	-
2	TYR	B	339	-	12,13,13	0.72	1 (8%)	13,17,17	0.80	1 (7%)
2	TYR	A	339	-	12,13,13	0.71	1 (8%)	13,17,17	0.73	1 (7%)
2	TYR	A	340	-	12,13,13	0.74	1 (8%)	13,17,17	0.75	1 (7%)
3	AZI	B	341	-	2,2,2	3.22	2 (100%)	0,1,1	-	-
2	TYR	D	339	-	12,13,13	0.70	1 (8%)	13,17,17	0.76	1 (7%)
3	AZI	A	341	-	2,2,2	3.23	2 (100%)	0,1,1	-	-
2	TYR	C	339	-	12,13,13	0.73	1 (8%)	13,17,17	0.75	1 (7%)
4	NO3	F	339	-	1,3,3	3.18	1 (100%)	0,3,3	-	-
2	TYR	C	340	-	12,13,13	0.73	1 (8%)	13,17,17	0.72	1 (7%)
2	TYR	H	339	-	12,13,13	0.74	1 (8%)	13,17,17	0.77	1 (7%)
2	TYR	B	340	-	12,13,13	0.71	1 (8%)	13,17,17	0.74	1 (7%)
4	NO3	A	342	-	1,3,3	3.08	1 (100%)	0,3,3	-	-

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	TYR	B	339	-	-	1/8/8/8	0/1/1/1
2	TYR	A	339	-	-	0/8/8/8	0/1/1/1
2	TYR	A	340	-	-	0/8/8/8	0/1/1/1
2	TYR	D	339	-	-	1/8/8/8	0/1/1/1
2	TYR	C	339	-	-	0/8/8/8	0/1/1/1
2	TYR	C	340	-	-	1/8/8/8	0/1/1/1
2	TYR	H	339	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYR	B	340	-	-	0/8/8/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	341	AZI	N3-N2	-3.25	1.16	1.23
3	A	341	AZI	N1-N2	-3.24	1.16	1.23
3	A	341	AZI	N3-N2	-3.23	1.16	1.23
4	D	340	NO3	O1-N	3.22	1.40	1.24
3	B	341	AZI	N1-N2	-3.20	1.16	1.23
4	F	339	NO3	O1-N	3.18	1.40	1.24
4	C	341	NO3	O1-N	3.17	1.39	1.24
4	A	342	NO3	O1-N	3.08	1.39	1.24
2	A	340	TYR	OXT-C	-2.31	1.23	1.30
2	C	340	TYR	OXT-C	-2.26	1.23	1.30
2	H	339	TYR	OXT-C	-2.25	1.23	1.30
2	B	339	TYR	OXT-C	-2.25	1.23	1.30
2	C	339	TYR	OXT-C	-2.24	1.23	1.30
2	D	339	TYR	OXT-C	-2.21	1.23	1.30
2	B	340	TYR	OXT-C	-2.20	1.23	1.30
2	A	339	TYR	OXT-C	-2.18	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	339	TYR	OXT-C-O	-2.81	117.71	124.08
2	H	339	TYR	OXT-C-O	-2.71	117.93	124.08
2	D	339	TYR	OXT-C-O	-2.64	118.08	124.08
2	A	340	TYR	OXT-C-O	-2.62	118.13	124.08
2	C	339	TYR	OXT-C-O	-2.60	118.19	124.08
2	B	340	TYR	OXT-C-O	-2.59	118.19	124.08
2	A	339	TYR	OXT-C-O	-2.57	118.24	124.08
2	C	340	TYR	OXT-C-O	-2.51	118.39	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	339	TYR	O-C-CA-N
2	D	339	TYR	O-C-CA-N
2	C	340	TYR	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	341	NO3	2	0
4	D	340	NO3	2	0
3	B	341	AZI	1	0
2	D	339	TYR	1	0
4	F	339	NO3	2	0
4	A	342	NO3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	338/338 (100%)	-0.22	10 (2%) 52 59	16, 35, 73, 166	0
1	B	338/338 (100%)	-0.27	3 (0%) 81 84	17, 35, 57, 93	0
1	C	338/338 (100%)	0.04	14 (4%) 41 47	18, 35, 73, 148	1 (0%)
1	D	338/338 (100%)	-0.08	9 (2%) 56 63	21, 42, 64, 120	0
1	E	338/338 (100%)	-0.11	8 (2%) 59 66	17, 39, 62, 139	0
1	F	338/338 (100%)	-0.11	11 (3%) 49 56	18, 39, 67, 127	0
1	G	338/338 (100%)	0.10	10 (2%) 52 59	17, 37, 61, 115	1 (0%)
1	H	338/338 (100%)	0.29	10 (2%) 52 59	20, 45, 68, 110	0
All	All	2704/2704 (100%)	-0.05	75 (2%) 55 61	16, 38, 66, 166	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	5.1
1	G	134	THR	5.0
1	A	134	THR	4.9
1	C	137	TYR	4.7
1	A	135	SER	4.4
1	C	136	PRO	4.3
1	E	137	TYR	4.2
1	F	137	TYR	4.1
1	C	130	TYR	3.9
1	C	134	THR	3.9
1	D	134	THR	3.8
1	E	136	PRO	3.8
1	E	134	THR	3.6
1	A	136	PRO	3.6
1	H	140	GLN	3.6
1	D	139	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	132	PRO	3.6
1	G	136	PRO	3.4
1	H	136	PRO	3.3
1	G	245	ALA	3.3
1	F	136	PRO	3.3
1	E	135	SER	3.3
1	E	138	SER	3.2
1	C	135	SER	3.1
1	A	139	PHE	3.1
1	D	136	PRO	3.1
1	C	141	GLY	2.9
1	G	47	TYR	2.9
1	F	92	ASN	2.9
1	H	310	GLY	2.9
1	G	133	ARG	2.9
1	C	140	GLN	2.8
1	D	138	SER	2.8
1	E	245	ALA	2.8
1	H	245	ALA	2.8
1	A	138	SER	2.8
1	G	137	TYR	2.7
1	D	132	PRO	2.7
1	A	137	TYR	2.6
1	H	137	TYR	2.6
1	F	132	PRO	2.6
1	D	137	TYR	2.6
1	F	246	THR	2.6
1	A	76	PHE	2.6
1	C	166	LEU	2.5
1	F	139	PHE	2.5
1	C	142	LEU	2.5
1	G	135	SER	2.5
1	G	132	PRO	2.5
1	G	191	PHE	2.5
1	F	134	THR	2.4
1	C	191	PHE	2.4
1	E	133	ARG	2.4
1	H	133	ARG	2.4
1	C	138	SER	2.4
1	F	76	PHE	2.4
1	D	140	GLN	2.3
1	B	136	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	135	SER	2.3
1	B	133	ARG	2.3
1	C	139	PHE	2.3
1	E	132	PRO	2.3
1	A	133	ARG	2.3
1	B	135	SER	2.3
1	G	246	THR	2.2
1	H	169	ASP	2.2
1	F	135	SER	2.2
1	H	311	LYS	2.2
1	C	131	LYS	2.1
1	D	247	ARG	2.1
1	F	133	ARG	2.1
1	H	149	TYR	2.1
1	A	132	PRO	2.1
1	A	131	LYS	2.0
1	H	321	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AZI	A	341	3/3	0.85	0.13	71,71,72,72	0
3	AZI	B	341	3/3	0.89	0.11	78,78,79,79	0
5	CL	B	342	1/1	0.90	0.16	66,66,66,66	0
4	NO3	C	341	4/4	0.93	0.09	36,36,38,41	0
2	TYR	B	340	13/13	0.93	0.07	22,29,35,36	0
2	TYR	H	339	13/13	0.95	0.06	25,29,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NO3	D	340	4/4	0.95	0.10	37,38,39,42	0
4	NO3	F	339	4/4	0.95	0.08	28,29,31,32	0
4	NO3	A	342	4/4	0.95	0.07	29,31,34,35	0
2	TYR	C	339	13/13	0.96	0.06	17,20,26,27	0
2	TYR	B	339	13/13	0.96	0.06	18,25,31,34	0
2	TYR	A	340	13/13	0.96	0.06	24,27,32,36	0
2	TYR	C	340	13/13	0.97	0.05	21,23,26,26	0
2	TYR	D	339	13/13	0.97	0.05	27,30,35,40	0
2	TYR	A	339	13/13	0.98	0.05	18,20,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.