



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:07 AM UTC

PDB ID : 7TGJ / pdb_00007tgj
Title : Crystal structure of DesD, the desferrioxamine synthetase from the Streptomyces griseoflavus ferrimycin biosynthetic pathway
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2022-01-07
Resolution : 2.85 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

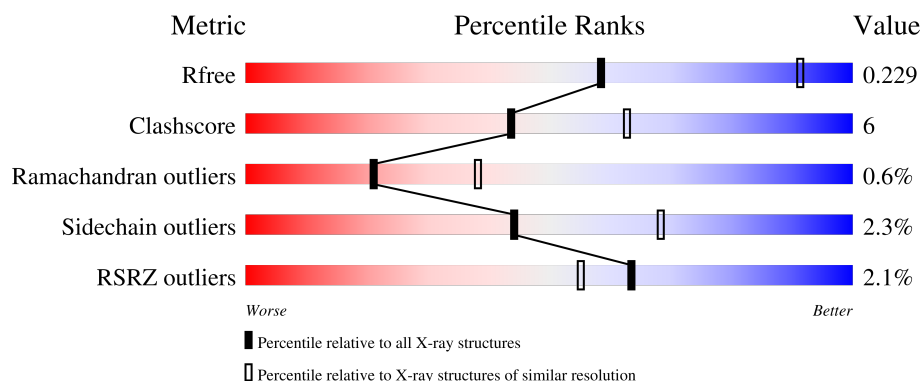
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	612	2% 80% 15% 5%
1	B	612	2% 79% 14% • 5%
1	C	612	2% 81% 13% • 5%
1	D	612	2% 75% 19% • 5%
1	E	612	2% 81% 14% 5%

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
2	GOL	B	601	-	X	-	-
2	GOL	C	604	-	X	-	-
3	SO4	A	608	-	-	X	-

2 Entry composition [i](#)

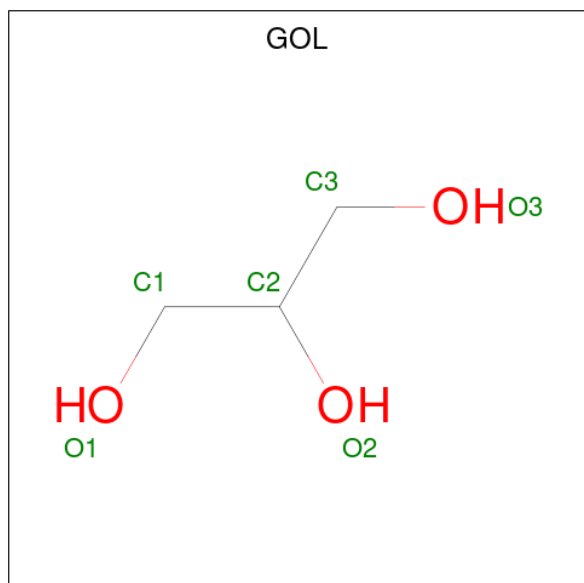
There are 4 unique types of molecules in this entry. The entry contains 22979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Desferrioxamine synthetase DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4558	2909	791	844	14			
1	B	580	Total	C	N	O	S	0	1	0
			4561	2911	791	844	15			
1	C	580	Total	C	N	O	S	0	0	0
			4538	2898	783	842	15			
1	D	579	Total	C	N	O	S	0	1	0
			4499	2879	774	832	14			
1	E	581	Total	C	N	O	S	0	0	0
			4512	2886	780	832	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



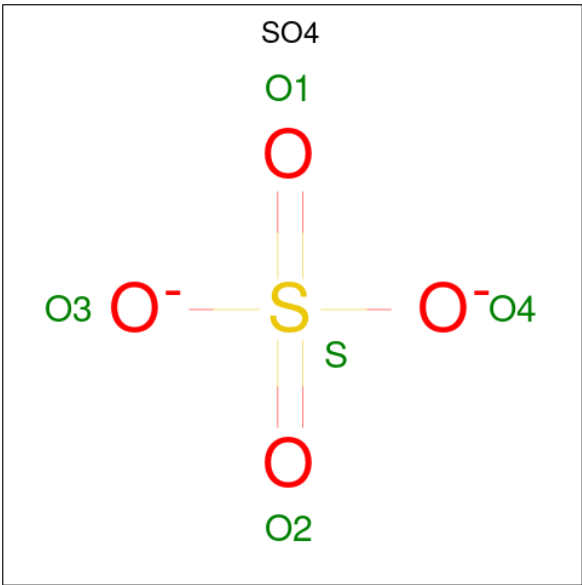
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

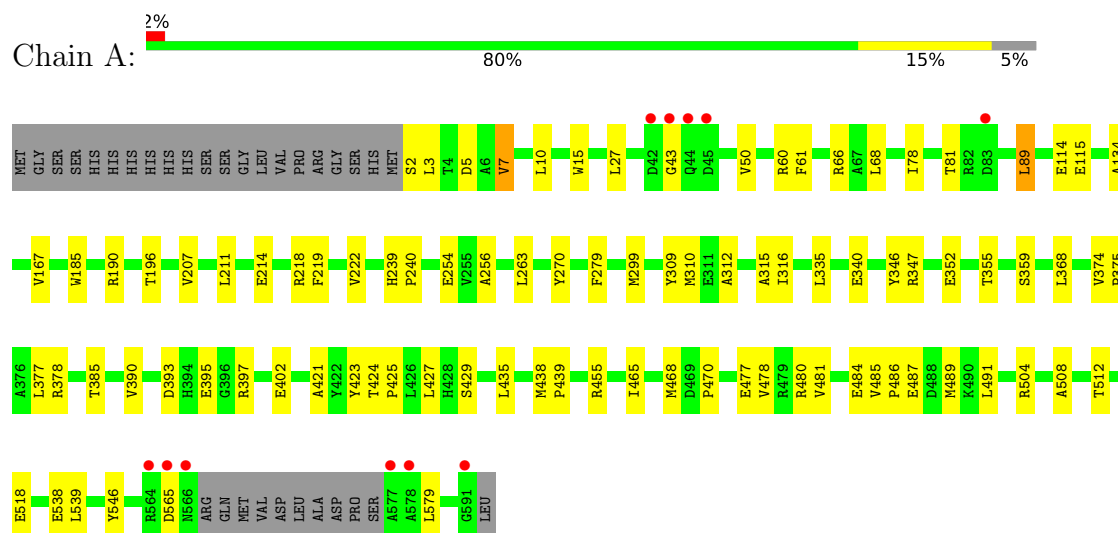
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	20	Total	O	0	0
			20	20		
4	C	18	Total	O	0	0
			18	18		
4	D	14	Total	O	0	0
			14	14		
4	E	12	Total	O	0	0
			12	12		

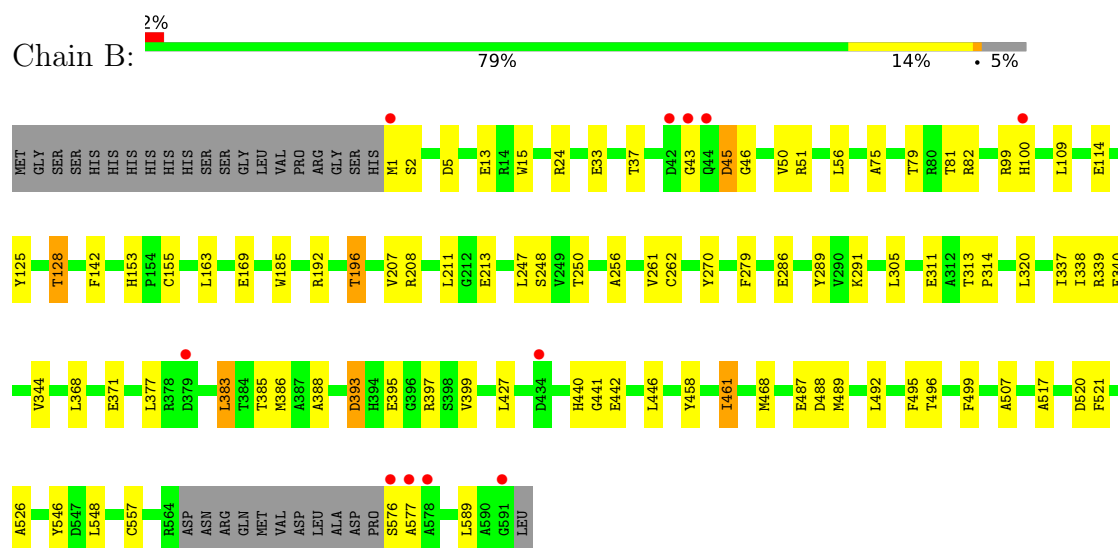
3 Residue-property plots

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.

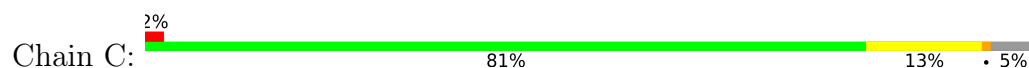
• Molecule 1: Desferrioxamine synthetase DesD

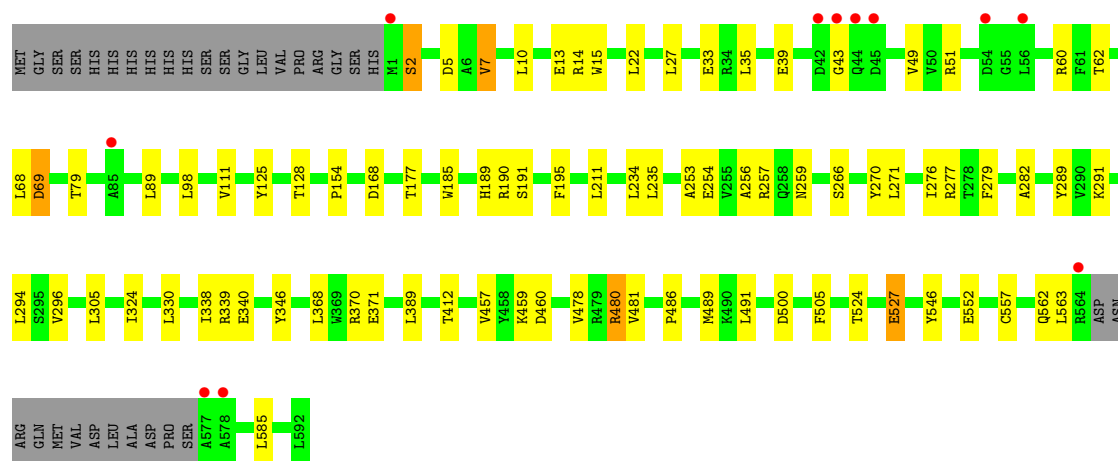


• Molecule 1: Desferrioxamine synthetase DesD

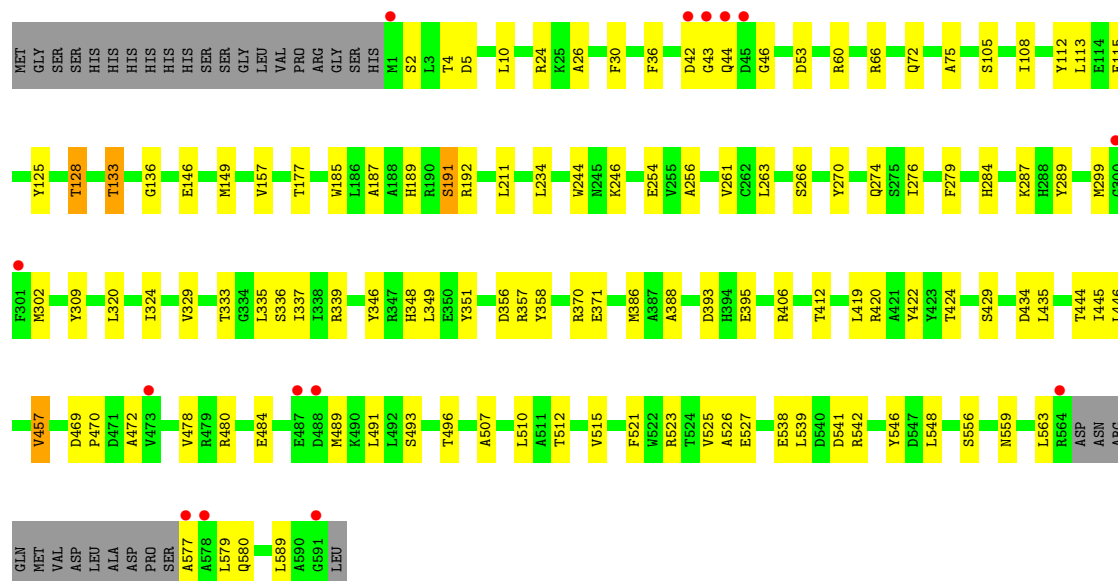
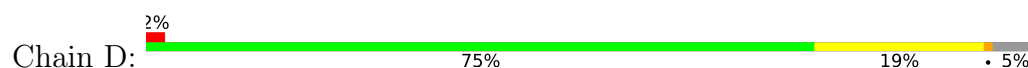


• Molecule 1: Desferrioxamine synthetase DesD

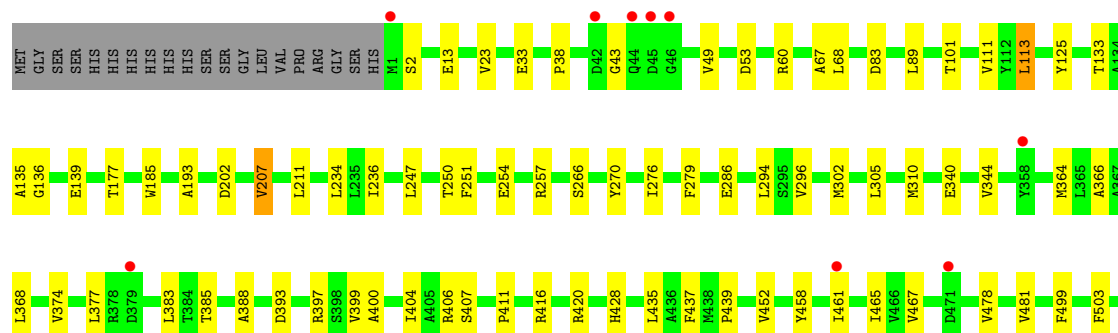
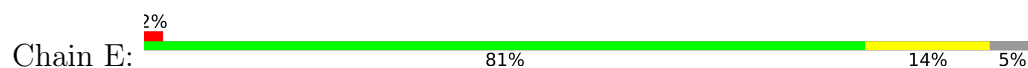


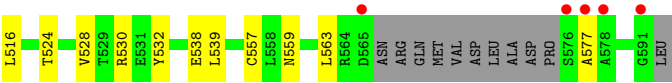


• Molecule 1: Desferrioxamine synthetase DesD



• Molecule 1: Desferrioxamine synthetase DesD





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.10Å 238.49Å 327.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.97 – 2.85 81.97 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (81.97-2.85) 93.6 (81.97-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.221 0.192 , 0.229	Depositor DCC
R_{free} test set	5404 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22979	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: GOL, SO4

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	0.42	0/4670	0.61	0/6361
1	B	0.44	0/4677	0.62	1/6371 (0.0%)
1	C	0.39	0/4650	0.58	0/6335
1	D	0.38	0/4615	0.58	0/6297
1	E	0.37	0/4624	0.55	0/6307
All	All	0.40	0/23236	0.59	1/31671 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	289	TYR	CA-CB-CG	5.53	123.86	113.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4558	0	4426	60	0
1	B	4561	0	4433	55	0
1	C	4538	0	4394	54	0
1	D	4499	0	4337	72	0
1	E	4512	0	4356	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	18	0	24	1	0
2	B	18	0	24	3	0
2	C	30	0	40	3	0
2	D	12	0	16	0	0
2	E	6	0	8	0	0
3	A	40	0	0	2	0
3	B	30	0	0	1	0
3	C	30	0	0	1	0
3	D	20	0	0	1	0
3	E	15	0	0	0	0
4	A	28	0	0	0	0
4	B	20	0	0	1	0
4	C	18	0	0	1	0
4	D	14	0	0	2	0
4	E	12	0	0	0	0
All	All	22979	0	22058	276	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 6.

All (276) 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:393:ASP:HB3	1:B:395:GLU:H	1.37	0.89
1:A:486:PRO:HG2	1:A:489:MET:HE3	1.54	0.88
1:D:489:MET:HE1	1:D:577:ALA:N	1.93	0.83
1:E:133:THR:HB	1:E:136:GLY:H	1.45	0.81
1:A:470:PRO:HG3	1:A:484:GLU:HG2	1.67	0.77
1:C:486:PRO:HG2	1:C:489:MET:HE2	1.67	0.77
1:A:340:GLU:HG2	1:A:368:LEU:HD13	1.69	0.74
1:A:397:ARG:HD3	1:A:402:GLU:HG2	1.67	0.74
1:A:115:GLU:HG3	1:A:299:MET:HE2	1.71	0.72
1:D:189:HIS:ND1	1:D:191:SER:HB3	2.05	0.70
1:D:445:ILE:HB	1:D:457:VAL:HG22	1.75	0.68
1:D:419:LEU:HD11	1:D:525:VAL:HG22	1.76	0.68
1:D:523:ARG:O	1:D:527:GLU:HG3	1.94	0.67
1:A:7:VAL:HG22	1:A:10:LEU:HD12	1.75	0.67
1:A:393:ASP:HB3	1:A:395:GLU:H	1.60	0.67
1:A:468:MET:HG2	1:A:485:VAL:HG21	1.77	0.67
1:B:196:THR:HG21	1:B:311:GLU:HA	1.76	0.66
1:D:270:TYR:HB3	1:D:279:PHE:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:HB2	1:C:234:LEU:HD23	1.78	0.66
1:D:72:GLN:NE2	1:D:512:THR:OG1	2.25	0.65
1:D:133:THR:HG23	1:D:136:GLY:H	1.61	0.65
1:D:146:GLU:OE1	1:D:274:GLN:HG3	1.96	0.65
1:C:277:ARG:NH1	1:C:291:LYS:HE3	2.12	0.65
1:A:310:MET:HA	1:A:310:MET:HE2	1.80	0.64
1:B:185:TRP:CZ2	1:B:211:LEU:HD11	2.32	0.64
1:C:277:ARG:HH11	1:C:291:LYS:HE3	1.62	0.64
1:D:125:TYR:CE2	1:D:177:THR:HG22	2.33	0.64
1:C:7:VAL:HG22	1:C:10:LEU:HD12	1.80	0.63
1:A:270:TYR:HB3	1:A:279:PHE:HB3	1.80	0.63
1:D:386:MET:HE1	1:D:422:TYR:CD1	2.32	0.63
1:E:193:ALA:HB1	1:E:234:LEU:HD11	1.81	0.63
1:A:27:LEU:HD12	1:A:78:ILE:HD13	1.79	0.62
1:C:49:VAL:HG23	1:C:60:ARG:HG2	1.80	0.62
1:D:309:TYR:HE1	1:D:480:ARG:HG2	1.62	0.62
1:E:185:TRP:CE2	1:E:211:LEU:HD21	2.35	0.62
1:B:99:ARG:HG3	1:B:109:LEU:HD22	1.80	0.62
1:D:185:TRP:CZ2	1:D:211:LEU:HD21	2.34	0.62
1:E:458:TYR:HB3	1:E:461:ILE:HD11	1.81	0.62
1:D:393:ASP:HB3	1:D:395:GLU:H	1.65	0.62
1:D:491:LEU:HD21	1:D:548:LEU:HD23	1.82	0.61
1:E:340:GLU:HG2	1:E:368:LEU:HD13	1.82	0.61
1:A:2:SER:HA	1:A:5:ASP:HB2	1.82	0.61
1:E:236:ILE:HG12	1:E:344:VAL:HG21	1.83	0.61
1:B:489:MET:HE3	1:B:576:SER:HB2	1.83	0.61
1:C:340:GLU:HG2	1:C:368:LEU:HD13	1.82	0.61
1:C:190:ARG:HG2	1:C:234:LEU:CD1	2.31	0.61
1:A:66:ARG:NH1	1:A:518:GLU:OE2	2.33	0.60
1:E:53:ASP:OD1	1:E:101:THR:OG1	2.20	0.59
1:D:386:MET:HE2	1:D:446:LEU:HD21	1.85	0.59
1:A:393:ASP:HB2	1:A:397:ARG:H	1.68	0.59
1:A:478:VAL:O	1:A:481:VAL:HG22	2.03	0.59
1:D:192:ARG:HG2	1:D:349:LEU:HD13	1.85	0.59
1:E:388:ALA:O	1:E:399:VAL:HB	2.04	0.58
1:E:305:LEU:HD22	1:E:310:MET:HE3	1.86	0.58
1:D:526:ALA:HB2	1:D:589:LEU:HD22	1.86	0.58
1:B:488:ASP:OD1	1:B:488:ASP:N	2.36	0.57
1:D:538:GLU:HG2	1:D:539:LEU:HG	1.86	0.57
1:B:386:MET:HE2	1:B:441:GLY:HA2	1.85	0.57
1:C:270:TYR:HB3	1:C:279:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:LEU:HD11	1:E:383:LEU:HG	1.85	0.57
1:D:339:ARG:NH2	1:D:371:GLU:OE2	2.31	0.57
1:B:208:ARG:NH1	1:B:213:GLU:OE2	2.38	0.57
1:E:270:TYR:HB3	1:E:279:PHE:HB3	1.87	0.57
1:E:524:THR:O	1:E:528:VAL:HG23	2.05	0.57
1:E:400:ALA:O	1:E:404:ILE:HG13	2.05	0.56
1:A:421:ALA:HB1	1:A:455:ARG:HA	1.85	0.56
1:D:336:SER:O	1:D:457:VAL:HA	2.05	0.56
1:C:2:SER:HB3	1:C:5:ASP:HB2	1.87	0.56
1:D:2:SER:HB3	1:D:5:ASP:HB2	1.87	0.55
1:D:470:PRO:HG3	1:D:484:GLU:HA	1.89	0.55
1:C:190:ARG:HG2	1:C:234:LEU:HD12	1.89	0.55
1:D:66:ARG:NE	1:D:72:GLN:OE1	2.36	0.55
1:B:51:ARG:H	2:B:602:GOL:H2	1.72	0.54
1:B:43:GLY:O	1:C:480:ARG:HB3	2.07	0.54
1:E:435:LEU:HG	1:E:465:ILE:HD11	1.88	0.54
1:E:13:GLU:CD	1:E:13:GLU:H	2.15	0.54
1:A:491:LEU:HD22	1:A:546:TYR:HB3	1.88	0.54
1:C:253:ALA:O	1:C:257:ARG:HG3	2.08	0.54
1:A:134:ALA:N	1:A:393:ASP:OD2	2.40	0.54
1:C:13:GLU:CD	1:C:13:GLU:H	2.16	0.53
1:D:356:ASP:OD2	1:D:358:TYR:N	2.34	0.53
1:E:530:ARG:HG2	1:E:530:ARG:HH11	1.72	0.53
1:D:320:LEU:O	1:D:324:ILE:HG12	2.08	0.53
1:A:393:ASP:HB3	1:A:395:GLU:N	2.24	0.53
1:D:112:TYR:HA	1:D:299:MET:HE1	1.91	0.53
1:C:562:GLN:O	1:C:563:LEU:HD23	2.09	0.53
1:C:185:TRP:HE1	1:C:266:SER:HB3	1.73	0.53
1:D:115:GLU:HG3	1:D:299:MET:CE	2.39	0.52
1:E:393:ASP:HB2	1:E:397:ARG:O	2.09	0.52
1:B:13:GLU:CD	1:B:13:GLU:H	2.17	0.52
1:D:254:GLU:OE2	1:D:346:TYR:OH	2.25	0.52
1:C:15:TRP:HB2	1:D:256:ALA:HB1	1.91	0.52
1:C:235:LEU:HD21	2:C:605:GOL:H2	1.92	0.52
1:D:289:TYR:HB2	1:D:370:ARG:HB3	1.92	0.52
1:C:14:ARG:HH22	2:C:604:GOL:H32	1.74	0.51
1:E:139:GLU:OE1	1:E:406:ARG:NH2	2.34	0.51
1:A:68:LEU:HD12	1:A:504:ARG:HB2	1.92	0.51
1:C:125:TYR:CE2	1:C:177:THR:HG22	2.46	0.51
1:E:133:THR:HG22	1:E:135:ALA:H	1.76	0.51
1:A:429:SER:HB3	1:A:435:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:GLU:HG2	1:E:368:LEU:CD1	2.40	0.51
1:B:100[B]:HIS:HE1	1:D:53:ASP:HB3	1.76	0.51
1:C:69:ASP:HB2	1:C:585:LEU:HD21	1.93	0.51
1:B:192:ARG:NH1	4:B:702:HOH:O	2.43	0.51
1:D:60:ARG:NH2	3:D:604:SO4:O2	2.43	0.50
1:B:492:LEU:O	1:B:496:THR:HB	2.12	0.50
1:C:291:LYS:HE2	1:C:305:LEU:HD13	1.93	0.50
4:C:702:HOH:O	1:D:302:MET:HE1	2.11	0.50
1:A:315:ALA:HB1	1:A:477:GLU:HG3	1.93	0.50
1:D:320:LEU:HD23	1:D:337:ILE:HG21	1.92	0.50
1:D:185:TRP:HE1	1:D:266:SER:HB3	1.77	0.50
1:D:469:ASP:HB3	1:D:472:ALA:HB2	1.94	0.50
1:B:1:MET:HE3	1:B:1:MET:HA	1.92	0.50
1:D:386:MET:HE3	1:D:444:THR:HB	1.93	0.50
1:E:559:ASN:O	1:E:563:LEU:HG	2.11	0.50
1:E:478:VAL:O	1:E:481:VAL:HG22	2.12	0.49
1:D:491:LEU:HD22	1:D:546:TYR:HB3	1.94	0.49
1:E:305:LEU:HB3	1:E:366:ALA:HB3	1.94	0.49
1:C:289:TYR:HB2	1:C:370:ARG:HB3	1.95	0.49
1:E:538:GLU:HG2	1:E:539:LEU:HG	1.94	0.49
1:B:50:VAL:HA	2:B:602:GOL:H31	1.94	0.49
1:C:125:TYR:CZ	1:C:177:THR:HG22	2.48	0.49
1:C:14:ARG:NE	1:C:128:THR:HG22	2.28	0.49
1:C:190:ARG:HG2	1:C:234:LEU:HD11	1.95	0.49
1:C:338:ILE:HG23	1:C:457:VAL:HG11	1.94	0.49
1:A:435:LEU:HD11	1:A:465:ILE:HD11	1.93	0.49
1:D:496:THR:HG21	1:D:556:SER:HB3	1.95	0.48
1:D:434:ASP:OD1	1:D:542:ARG:NH2	2.46	0.48
1:B:169:GLU:OE2	2:B:601:GOL:H32	2.13	0.48
1:A:185:TRP:CE2	1:A:211:LEU:HD21	2.49	0.48
1:D:115:GLU:HG3	1:D:299:MET:HE3	1.94	0.48
1:B:100[B]:HIS:CE1	1:D:53:ASP:HB3	2.48	0.48
1:A:347:ARG:HD2	1:A:352:GLU:OE2	2.13	0.47
1:C:460:ASP:HB2	3:C:608:SO4:O2	2.13	0.47
1:B:125:TYR:O	1:B:128:THR:HB	2.14	0.47
1:B:270:TYR:HB3	1:B:279:PHE:HB3	1.94	0.47
1:C:39:GLU:HG2	1:C:49:VAL:HG12	1.97	0.47
1:A:114:GLU:HG3	1:B:250:THR:HG23	1.96	0.47
1:A:15:TRP:HB2	1:B:256:ALA:HB1	1.95	0.47
1:E:416:ARG:HD2	1:E:420:ARG:NH2	2.29	0.47
1:D:133:THR:HG23	1:D:136:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:OE2	1:A:546:TYR:OH	2.31	0.47
1:D:24:ARG:HD3	1:D:75:ALA:HB2	1.97	0.47
1:B:2:SER:HB3	1:B:5:ASP:HB2	1.97	0.47
1:B:377:LEU:HD11	1:B:383:LEU:HD22	1.95	0.47
1:A:219:PHE:CG	1:A:263:LEU:HD13	2.50	0.46
1:C:254:GLU:OE1	1:C:346:TYR:OH	2.30	0.46
1:C:524:THR:HA	1:C:527:GLU:HG3	1.96	0.46
1:E:411:PRO:HB2	1:E:516:LEU:HD13	1.96	0.46
1:D:125:TYR:O	1:D:128:THR:HB	2.16	0.46
1:E:23:VAL:HG11	1:E:89:LEU:HD11	1.98	0.46
1:E:286:GLU:HG2	1:E:374:VAL:CG2	2.45	0.46
1:A:538:GLU:HG2	1:A:539:LEU:HG	1.98	0.46
1:B:340:GLU:HG2	1:B:368:LEU:HD13	1.96	0.46
1:D:187:ALA:HB3	1:D:261:VAL:HB	1.97	0.46
1:E:435:LEU:HD12	1:E:467:VAL:HG22	1.98	0.46
1:B:388:ALA:O	1:B:399:VAL:HB	2.15	0.46
1:A:315:ALA:CB	1:A:477:GLU:HG3	2.45	0.46
1:B:24:ARG:HD3	1:B:75:ALA:HB2	1.98	0.46
1:B:517:ALA:HB3	1:B:520:ASP:OD2	2.16	0.46
1:C:324:ILE:HG23	1:C:330:LEU:HB3	1.98	0.46
1:D:26:ALA:HA	1:D:157:VAL:HG21	1.98	0.46
1:D:246:LYS:HA	1:D:246:LYS:HD2	1.78	0.45
1:A:3:LEU:HG	1:B:262:CYS:SG	2.56	0.45
1:A:438:MET:HA	1:A:438:MET:HE2	1.99	0.45
1:B:386:MET:HG3	1:B:446:LEU:HD11	1.97	0.45
1:C:185:TRP:CZ2	1:C:211:LEU:HD21	2.52	0.45
1:C:257:ARG:HD2	2:C:602:GOL:H32	1.98	0.45
1:A:214:GLU:H	1:A:214:GLU:CD	2.25	0.45
1:A:239:HIS:ND1	1:A:240:PRO:HD2	2.32	0.45
1:C:294:LEU:HG	1:C:296:VAL:HG13	1.97	0.45
1:E:185:TRP:HE1	1:E:266:SER:HB3	1.82	0.45
1:B:291:LYS:HE3	3:B:607:SO4:O4	2.17	0.45
1:C:338:ILE:HD11	1:C:459:LYS:HB3	1.98	0.45
1:C:491:LEU:HD22	1:C:546:TYR:HB3	1.99	0.45
1:D:429:SER:HB3	1:D:435:LEU:HD23	1.99	0.45
1:D:335:LEU:HG	1:D:336:SER:N	2.33	0.44
1:C:271:LEU:HG	1:C:282:ALA:HB2	1.99	0.44
1:C:68:LEU:HD13	1:C:500:ASP:HA	1.99	0.44
1:E:133:THR:HB	1:E:136:GLY:N	2.23	0.44
1:E:33:GLU:OE1	1:E:557:CYS:HB3	2.18	0.44
1:A:50:VAL:HG23	1:A:61:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:MET:HE1	1:E:364:MET:CE	2.47	0.44
1:B:286:GLU:H	1:B:286:GLU:CD	2.24	0.44
1:B:495:PHE:O	1:B:499:PHE:HB2	2.17	0.44
1:A:335:LEU:HD22	1:A:425:PRO:HB3	1.99	0.44
1:A:355:THR:HB	1:A:359:SER:HB2	2.00	0.44
1:A:468:MET:HE3	1:A:468:MET:HB2	1.84	0.44
1:D:420:ARG:HA	1:D:424:THR:OG1	2.18	0.44
1:C:189:HIS:ND1	1:C:191:SER:HB3	2.33	0.44
1:E:207:VAL:HG13	1:E:211:LEU:HD12	1.99	0.44
1:D:4:THR:HG23	4:D:709:HOH:O	2.17	0.43
1:B:45:ASP:HB3	1:B:46:GLY:H	1.42	0.43
1:E:428:HIS:HA	1:E:532:TYR:OH	2.18	0.43
1:A:254:GLU:OE1	1:A:346:TYR:OH	2.33	0.43
1:B:313:THR:HB	1:B:314:PRO:HD3	2.00	0.43
1:C:291:LYS:HB3	1:C:368:LEU:HG	2.01	0.43
1:E:499:PHE:HA	1:E:503:PHE:HB2	1.99	0.43
1:A:60:ARG:HH21	2:A:603:GOL:H31	1.83	0.43
1:D:149:MET:HE2	1:D:149:MET:HA	2.01	0.43
1:D:149:MET:SD	1:D:388:ALA:HA	2.58	0.43
1:A:190:ARG:NH2	3:A:608:SO4:O2	2.51	0.43
1:A:477:GLU:CD	1:A:477:GLU:H	2.27	0.43
1:C:35:LEU:HD23	1:C:35:LEU:HA	1.84	0.43
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.84	0.43
1:A:218:ARG:O	1:A:222:VAL:HG23	2.19	0.43
1:B:393:ASP:HB2	1:B:397:ARG:H	1.84	0.43
1:E:125:TYR:CE2	1:E:177:THR:HG22	2.53	0.43
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.73	0.42
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.74	0.42
1:E:294:LEU:HG	1:E:296:VAL:HG13	2.01	0.42
1:C:69:ASP:HB2	1:C:585:LEU:CD2	2.49	0.42
1:D:320:LEU:HD23	1:D:337:ILE:HD13	2.01	0.42
1:E:247:LEU:O	1:E:251:PHE:HB2	2.20	0.42
1:D:510:LEU:HD22	1:D:515:VAL:HG11	2.02	0.42
1:B:320:LEU:HD23	1:B:461:ILE:HG13	2.02	0.42
1:C:168:ASP:HB3	1:D:244:TRP:CZ3	2.54	0.42
1:B:153:HIS:CE1	1:B:155:CYS:HB2	2.54	0.42
1:B:468:MET:HE3	1:B:468:MET:HB2	1.73	0.42
1:B:487:GLU:OE2	1:B:546:TYR:OH	2.27	0.42
1:A:66:ARG:HH21	1:A:512:THR:HG22	1.85	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.85	0.42
1:E:305:LEU:HD22	1:E:310:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:NH2	3:A:608:SO4:S	2.92	0.42
1:A:256:ALA:HB1	1:B:15:TRP:HB2	2.02	0.42
1:D:329:VAL:O	1:D:333:THR:HG23	2.19	0.42
1:D:579:LEU:O	1:D:580:GLN:HG2	2.20	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.83	0.42
1:C:339:ARG:NH2	1:C:371:GLU:OE2	2.35	0.42
1:B:427:LEU:HD23	1:B:427:LEU:HA	1.85	0.41
1:D:284:HIS:HB2	1:D:287:LYS:HD3	2.03	0.41
1:D:507:ALA:HB2	1:D:521:PHE:CD1	2.55	0.41
1:E:49:VAL:HG23	1:E:60:ARG:HG2	2.01	0.41
1:E:286:GLU:HG2	1:E:374:VAL:HG23	2.02	0.41
1:A:309:TYR:HE1	1:A:480:ARG:HD3	1.85	0.41
1:A:374:VAL:N	1:A:375:PRO:HD2	2.35	0.41
1:D:30:PHE:HB2	1:D:36:PHE:CZ	2.54	0.41
1:D:348:HIS:CG	1:D:351:TYR:HD2	2.38	0.41
1:D:559:ASN:O	1:D:563:LEU:HG	2.20	0.41
1:E:67:ALA:O	1:E:68:LEU:HB2	2.21	0.41
1:E:407:SER:HB2	1:E:452:VAL:HG23	2.03	0.41
1:B:339:ARG:NH2	1:B:371:GLU:OE2	2.37	0.41
1:A:424:THR:HB	1:A:425:PRO:HD3	2.02	0.41
1:B:305:LEU:HD12	1:B:305:LEU:HA	1.90	0.41
1:B:507:ALA:HB2	1:B:521:PHE:CD1	2.56	0.41
1:A:167:VAL:HB	1:B:248:SER:OG	2.21	0.41
1:A:347:ARG:NH1	1:A:352:GLU:OE1	2.54	0.41
1:B:33:GLU:OE1	1:B:557:CYS:HB3	2.20	0.41
1:B:114:GLU:HG2	1:B:163:LEU:HD11	2.01	0.41
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.78	0.41
1:C:33:GLU:OE1	1:C:557:CYS:HB3	2.21	0.41
1:D:105:SER:OG	1:D:108:ILE:HG22	2.21	0.41
1:D:187:ALA:HB2	1:D:263:LEU:HD11	2.02	0.41
1:E:113:LEU:HD12	1:E:113:LEU:HA	1.82	0.41
1:A:508:ALA:O	1:A:512:THR:HG23	2.21	0.41
1:C:168:ASP:HB3	1:D:244:TRP:CE3	2.56	0.41
1:C:259:ASN:HB3	1:C:346:TYR:OH	2.21	0.41
1:D:541:ASP:OD2	1:D:541:ASP:N	2.53	0.41
1:D:580:GLN:N	4:D:702:HOH:O	2.54	0.41
1:A:378:ARG:HA	1:A:378:ARG:HD2	1.83	0.40
1:C:478:VAL:O	1:C:481:VAL:HG22	2.21	0.40
1:A:423:TYR:CE2	1:A:427:LEU:HD11	2.56	0.40
1:B:526:ALA:HB2	1:B:589:LEU:HD22	2.02	0.40
1:C:27:LEU:HA	1:C:27:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:HG2	1:A:368:LEU:CD1	2.44	0.40
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.77	0.40
1:A:312:ALA:O	1:A:316:ILE:HG13	2.22	0.40
1:B:142:PHE:CD1	1:B:383:LEU:HB3	2.56	0.40
1:B:337:ILE:HG22	1:B:458:TYR:HB2	2.02	0.40
1:B:440:HIS:CE1	1:B:442:GLU:HB3	2.57	0.40
1:C:256:ALA:HB2	1:D:10:LEU:HB3	2.03	0.40
1:E:254:GLU:OE2	1:E:257:ARG:NH2	2.54	0.40
1:B:56:LEU:O	1:B:82:ARG:HG3	2.21	0.40
1:C:154:PRO:HB2	1:C:505:PHE:CZ	2.57	0.40
1:C:368:LEU:HD12	1:C:368:LEU:C	2.47	0.40
1:E:437:PHE:C	1:E:439:PRO:HD3	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/612 (94%)	552 (96%)	21 (4%)	3 (0%)	24	42
1	B	577/612 (94%)	546 (95%)	29 (5%)	2 (0%)	36	54
1	C	576/612 (94%)	546 (95%)	27 (5%)	3 (0%)	24	42
1	D	576/612 (94%)	550 (96%)	21 (4%)	5 (1%)	14	28
1	E	577/612 (94%)	548 (95%)	25 (4%)	4 (1%)	18	35
All	All	2882/3060 (94%)	2742 (95%)	123 (4%)	17 (1%)	21	38

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	ASP
1	A	43	GLY

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Mol	Chain	Res	Type
1	A	565	ASP
1	C	43	GLY
1	D	42	ASP
1	D	43	GLY
1	E	43	GLY
1	B	577	ALA
1	C	2	SER
1	D	46	GLY
1	E	577	ALA
1	D	44	GLN
1	E	276	ILE
1	C	276	ILE
1	A	439	PRO
1	E	38	PRO
1	D	276	ILE

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	465/504 (92%)	457 (98%)	8 (2%)	53	75
1	B	467/504 (93%)	454 (97%)	13 (3%)	38	62
1	C	461/504 (92%)	448 (97%)	13 (3%)	38	62
1	D	454/504 (90%)	444 (98%)	10 (2%)	45	69
1	E	454/504 (90%)	446 (98%)	8 (2%)	51	73
All	All	2301/2520 (91%)	2249 (98%)	52 (2%)	44	68

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	81	THR
1	A	89	LEU
1	A	196	THR

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Mol	Chain	Res	Type
1	A	207	VAL
1	A	385	THR
1	A	390	VAL
1	A	579	LEU
1	B	37	THR
1	B	45	ASP
1	B	79	THR
1	B	81	THR
1	B	128	THR
1	B	196	THR
1	B	207	VAL
1	B	261	VAL
1	B	338	ILE
1	B	344	VAL
1	B	383	LEU
1	B	385	THR
1	B	461	ILE
1	C	7	VAL
1	C	51	ARG
1	C	62	THR
1	C	69	ASP
1	C	79	THR
1	C	89	LEU
1	C	98	LEU
1	C	111	VAL
1	C	389	LEU
1	C	412	THR
1	C	480	ARG
1	C	527	GLU
1	C	552	GLU
1	D	128	THR
1	D	133	THR
1	D	191	SER
1	D	234	LEU
1	D	357	ARG
1	D	406	ARG
1	D	412	THR
1	D	457	VAL
1	D	478	VAL
1	D	493	SER
1	E	2	SER
1	E	83	ASP

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Mol	Chain	Res	Type
1	E	111	VAL
1	E	113	LEU
1	E	202	ASP
1	E	207	VAL
1	E	250	THR
1	E	385	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	245	ASN
1	A	284	HIS
1	A	545	GLN
1	B	131	GLN
1	B	160	ASN
1	C	391	HIS
1	C	454	GLN
1	C	580	GLN
1	D	160	ASN
1	D	417	HIS
1	D	533	GLN
1	D	580	GLN
1	E	209	GLN
1	E	284	HIS
1	E	298	ASN
1	E	454	GLN

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

41 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	GOL	D	602	-	5,5,5	2.06	2 (40%)	5,5,5	0.79	0
3	SO4	C	609	-	4,4,4	0.86	0	6,6,6	0.31	0
2	GOL	B	603	-	5,5,5	1.19	1 (20%)	5,5,5	1.23	0
2	GOL	A	603	-	5,5,5	0.97	0	5,5,5	0.98	0
3	SO4	E	602	-	4,4,4	0.65	0	6,6,6	0.51	0
3	SO4	B	604	-	4,4,4	0.72	0	6,6,6	0.22	0
3	SO4	B	607	-	4,4,4	0.46	0	6,6,6	0.68	0
3	SO4	A	605	-	4,4,4	0.70	0	6,6,6	0.38	0
3	SO4	A	608	-	4,4,4	0.81	0	6,6,6	0.30	0
3	SO4	A	604	-	4,4,4	0.54	0	6,6,6	0.26	0
3	SO4	A	611	-	4,4,4	0.90	0	6,6,6	0.24	0
3	SO4	B	606	-	4,4,4	0.63	0	6,6,6	0.45	0
3	SO4	B	608	-	4,4,4	0.88	0	6,6,6	0.35	0
2	GOL	A	602	-	5,5,5	1.14	1 (20%)	5,5,5	0.98	0
2	GOL	E	601	-	5,5,5	1.69	1 (20%)	5,5,5	1.27	0
3	SO4	A	609	-	4,4,4	0.42	0	6,6,6	0.37	0
3	SO4	A	607	-	4,4,4	0.72	0	6,6,6	0.30	0
3	SO4	E	603	-	4,4,4	0.55	0	6,6,6	0.33	0
3	SO4	C	606	-	4,4,4	0.72	0	6,6,6	0.54	0
3	SO4	D	605	-	4,4,4	0.55	0	6,6,6	0.50	0
3	SO4	D	606	-	4,4,4	0.78	0	6,6,6	0.33	0
2	GOL	A	601	-	5,5,5	1.25	1 (20%)	5,5,5	1.04	0
3	SO4	B	605	-	4,4,4	0.83	0	6,6,6	0.34	0
3	SO4	C	607	-	4,4,4	0.68	0	6,6,6	0.32	0
3	SO4	C	611	-	4,4,4	0.83	0	6,6,6	0.26	0
2	GOL	B	602	-	5,5,5	1.31	1 (20%)	5,5,5	1.35	1 (20%)
2	GOL	C	604	-	5,5,5	1.11	1 (20%)	5,5,5	1.55	1 (20%)
3	SO4	A	606	-	4,4,4	0.72	0	6,6,6	0.36	0
3	SO4	C	610	-	4,4,4	0.75	0	6,6,6	0.54	0
3	SO4	B	609	-	4,4,4	0.55	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	603	-	5,5,5	0.96	0	5,5,5	0.93	0
2	GOL	C	605	-	5,5,5	1.25	0	5,5,5	0.96	0
2	GOL	B	601	-	5,5,5	1.67	2 (40%)	5,5,5	1.11	1 (20%)
2	GOL	C	602	-	5,5,5	1.43	1 (20%)	5,5,5	1.29	0
3	SO4	D	604	-	4,4,4	0.87	0	6,6,6	0.32	0
2	GOL	C	601	-	5,5,5	1.13	0	5,5,5	0.93	0
3	SO4	D	603	-	4,4,4	0.69	0	6,6,6	0.35	0
3	SO4	E	604	-	4,4,4	0.84	0	6,6,6	0.33	0
2	GOL	D	601	-	5,5,5	1.94	2 (40%)	5,5,5	0.93	0
3	SO4	C	608	-	4,4,4	0.45	0	6,6,6	0.35	0
3	SO4	A	610	-	4,4,4	0.79	0	6,6,6	0.44	0

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	GOL	D	602	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	B	603	-	-	0/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	E	601	-	-	2/4/4/4	-
2	GOL	B	601	-	-	3/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	C	601	-	-	1/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	C	604	-	-	4/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	GOL	C1-C2	3.58	1.65	1.51
2	D	601	GOL	C1-C2	3.41	1.64	1.51
2	E	601	GOL	C1-C2	3.36	1.64	1.51
2	B	601	GOL	C1-C2	2.78	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	GOL	C3-C2	2.75	1.62	1.51
2	D	602	GOL	C3-C2	2.61	1.61	1.51
2	D	601	GOL	C3-C2	2.48	1.61	1.51
2	B	602	GOL	C3-C2	2.45	1.61	1.51
2	B	601	GOL	C3-C2	2.32	1.60	1.51
2	A	602	GOL	C1-C2	2.17	1.60	1.51
2	B	603	GOL	C1-C2	2.13	1.59	1.51
2	A	601	GOL	C1-C2	2.11	1.59	1.51
2	C	604	GOL	C3-C2	2.08	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	GOL	C3-C2-C1	-2.37	103.12	111.80
2	C	604	GOL	C3-C2-C1	-2.27	103.48	111.80
2	B	601	GOL	C3-C2-C1	-2.09	104.12	111.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	D	602	GOL	O1-C1-C2-C3
2	E	601	GOL	O1-C1-C2-O2
2	E	601	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-O2
2	A	603	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	C	604	GOL	O1-C1-C2-C3
2	C	604	GOL	C1-C2-C3-O3
2	C	605	GOL	O1-C1-C2-C3
2	C	605	GOL	O1-C1-C2-O2
2	B	602	GOL	O2-C2-C3-O3
2	C	604	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	C	601	GOL	O1-C1-C2-O2
2	D	602	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
2	C	604	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	GOL	1	0
3	B	607	SO4	1	0
3	A	608	SO4	2	0
2	B	602	GOL	2	0
2	C	604	GOL	1	0
2	C	605	GOL	1	0
2	B	601	GOL	1	0
2	C	602	GOL	1	0
3	D	604	SO4	1	0
3	C	608	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	580/612 (94%)	-0.33	11 (1%) 66 59	26, 45, 73, 116	0
1	B	580/612 (94%)	-0.36	11 (1%) 66 59	26, 43, 73, 104	1 (0%)
1	C	580/612 (94%)	-0.20	11 (1%) 66 59	35, 50, 75, 112	0
1	D	579/612 (94%)	-0.11	14 (2%) 59 51	30, 54, 84, 119	1 (0%)
1	E	581/612 (94%)	-0.07	14 (2%) 59 51	37, 57, 81, 120	0
All	All	2900/3060 (94%)	-0.22	61 (2%) 63 55	26, 50, 78, 120	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	ASN	6.9
1	C	577	ALA	6.4
1	E	577	ALA	6.0
1	E	591	GLY	5.9
1	C	42	ASP	5.5
1	E	45	ASP	4.8
1	B	42	ASP	4.6
1	A	45	ASP	4.6
1	D	44	GLN	4.5
1	A	591	GLY	4.3
1	C	578	ALA	4.2
1	E	42	ASP	4.2
1	C	54	ASP	4.2
1	A	565	ASP	4.2
1	A	577	ALA	4.1
1	E	565	ASP	4.1
1	D	591	GLY	4.1
1	C	45	ASP	4.0
1	E	471	ASP	3.9
1	B	591	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	577	ALA	3.8
1	A	42	ASP	3.8
1	E	576	SER	3.7
1	A	44	GLN	3.7
1	E	358	TYR	3.6
1	E	578	ALA	3.5
1	C	44	GLN	3.5
1	D	42	ASP	3.4
1	B	100[A]	HIS	3.3
1	B	44	GLN	3.3
1	B	577	ALA	3.2
1	A	83	ASP	3.2
1	D	45	ASP	3.1
1	E	46	GLY	3.0
1	D	473	VAL	3.0
1	B	578	ALA	3.0
1	C	85	ALA	3.0
1	B	434	ASP	2.9
1	B	43	GLY	2.9
1	A	564	ARG	2.9
1	E	44	GLN	2.9
1	D	43	GLY	2.7
1	A	43	GLY	2.5
1	D	564	ARG	2.4
1	D	1	MET	2.4
1	B	1	MET	2.3
1	E	379	ASP	2.2
1	B	576	SER	2.2
1	C	43	GLY	2.2
1	C	564	ARG	2.1
1	B	379	ASP	2.1
1	D	300	GLY	2.1
1	D	488	ASP	2.1
1	A	578	ALA	2.1
1	E	1	MET	2.0
1	C	56	LEU	2.0
1	D	301	PHE	2.0
1	C	1	MET	2.0
1	E	461	ILE	2.0
1	D	578	ALA	2.0
1	D	487	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($\text{\AA}^2$)	Q<0.9
2	GOL	C	601	6/6	0.70	0.21	75,81,81,85	0
2	GOL	C	604	6/6	0.74	0.17	57,61,66,66	0
2	GOL	C	602	6/6	0.75	0.23	53,60,62,65	0
2	GOL	B	603	6/6	0.77	0.19	58,62,64,65	0
2	GOL	A	601	6/6	0.80	0.18	65,69,74,79	0
2	GOL	A	603	6/6	0.83	0.15	72,75,75,76	0
2	GOL	D	601	6/6	0.84	0.16	51,57,58,58	0
3	SO4	A	607	5/5	0.85	0.27	68,73,78,82	0
2	GOL	B	602	6/6	0.86	0.20	47,48,51,53	0
2	GOL	C	605	6/6	0.86	0.23	58,59,65,65	0
3	SO4	C	606	5/5	0.86	0.23	68,75,77,82	0
3	SO4	E	604	5/5	0.86	0.24	72,74,84,88	0
3	SO4	A	605	5/5	0.87	0.20	61,63,78,78	0
3	SO4	A	608	5/5	0.87	0.30	58,64,77,79	0
3	SO4	C	611	5/5	0.88	0.18	66,69,75,79	0
2	GOL	C	603	6/6	0.88	0.14	56,58,59,62	0
3	SO4	A	611	5/5	0.89	0.26	64,65,76,79	0
3	SO4	D	606	5/5	0.89	0.21	73,74,77,84	0
2	GOL	E	601	6/6	0.89	0.16	46,48,55,60	0
3	SO4	D	603	5/5	0.90	0.19	65,66,76,79	0
3	SO4	D	604	5/5	0.90	0.19	62,64,67,79	0
2	GOL	B	601	6/6	0.91	0.12	41,43,47,49	0
3	SO4	C	609	5/5	0.91	0.28	65,65,75,77	0
2	GOL	D	602	6/6	0.91	0.14	45,47,48,51	0
3	SO4	A	610	5/5	0.91	0.27	59,64,74,76	0
3	SO4	A	606	5/5	0.91	0.15	52,54,63,65	0
3	SO4	B	604	5/5	0.91	0.26	60,61,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	605	5/5	0.91	0.21	65,65,69,80	0
3	SO4	C	607	5/5	0.92	0.18	55,56,67,70	0
3	SO4	B	609	5/5	0.92	0.18	62,64,68,70	0
3	SO4	C	610	5/5	0.92	0.13	62,62,67,72	0
3	SO4	B	608	5/5	0.92	0.17	65,66,73,81	0
3	SO4	E	602	5/5	0.93	0.15	55,57,66,67	0
3	SO4	D	605	5/5	0.94	0.10	60,61,68,69	0
2	GOL	A	602	6/6	0.95	0.09	38,39,41,46	0
3	SO4	A	604	5/5	0.95	0.10	54,55,57,59	0
3	SO4	E	603	5/5	0.95	0.12	59,60,64,65	0
3	SO4	C	608	5/5	0.95	0.14	54,54,60,60	0
3	SO4	B	607	5/5	0.96	0.13	45,49,53,54	0
3	SO4	A	609	5/5	0.97	0.07	50,51,55,56	0
3	SO4	B	606	5/5	0.97	0.10	49,51,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.