



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2022 – 12:21 PM EDT

PDB ID : 7TGJ  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

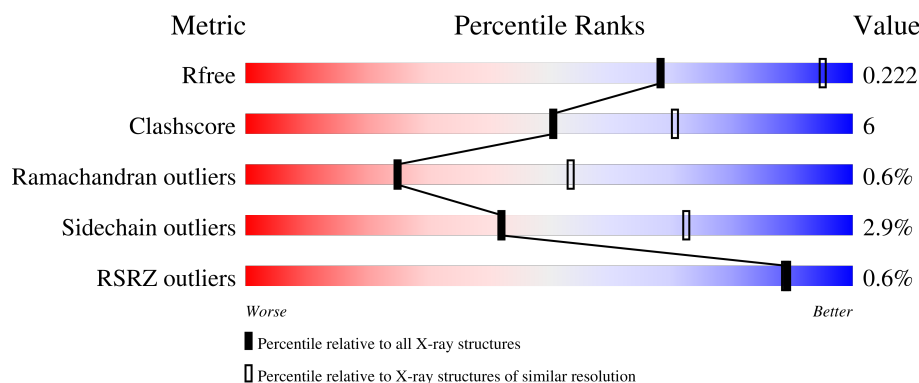
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	
1	B	612	
1	C	612	
1	D	612	
1	E	612	

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	-	-
3	SO4	A	608	-	-	X	-

## 2 Entry composition [i](#)

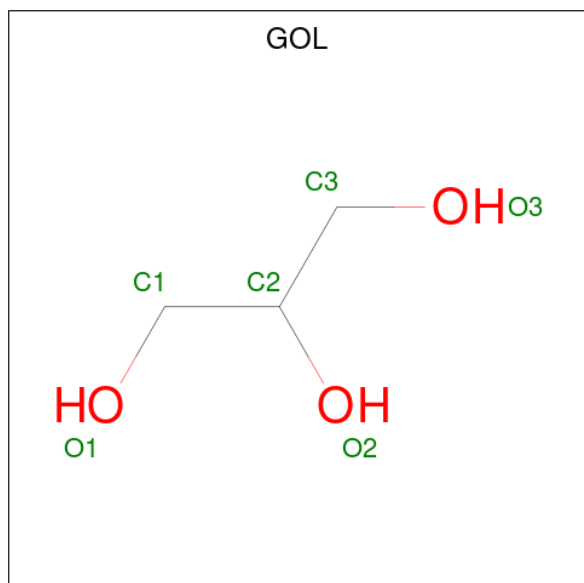
There are 4 unique types of molecules in this entry. The entry contains 22979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



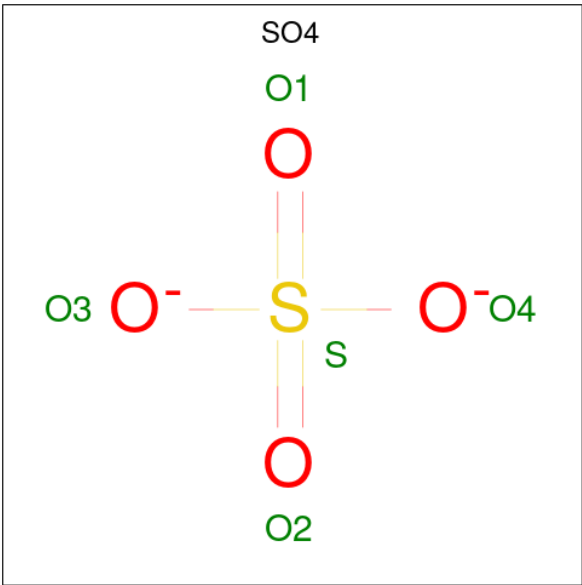
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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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	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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
			5	4	1		

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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		

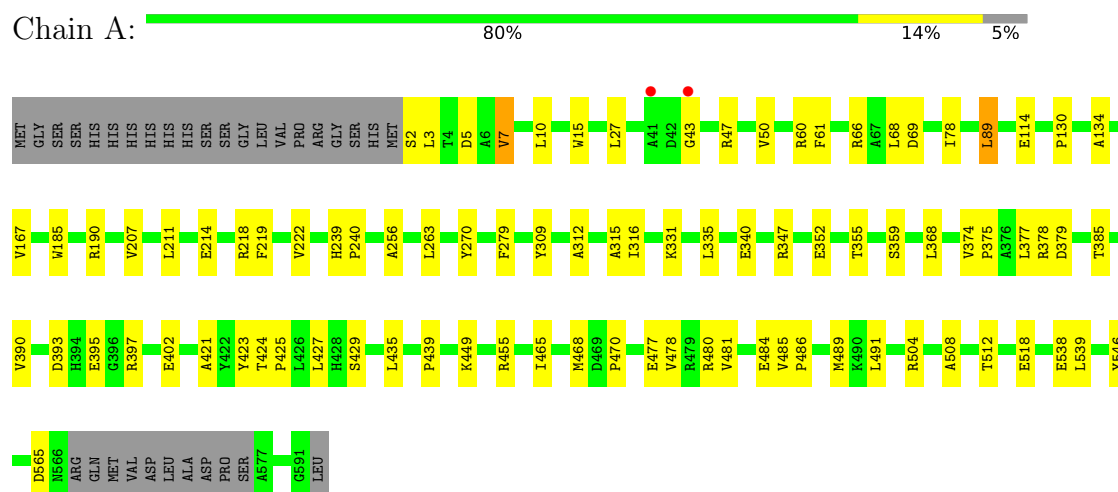
- Molecule 4 is water.

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		

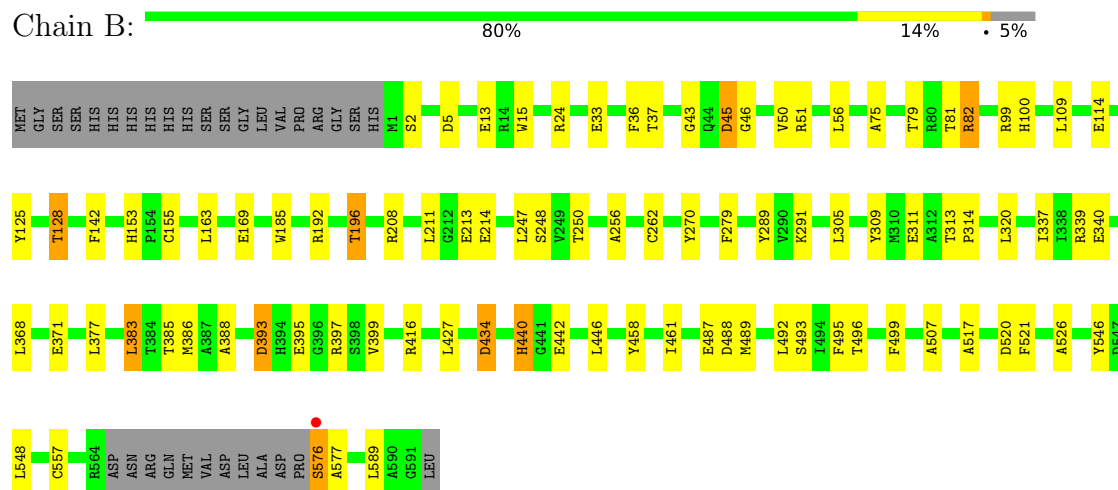
### 3 Residue-property plots

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.

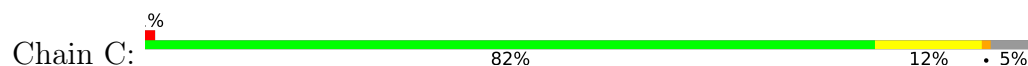
#### • Molecule 1: Desferrioxamine synthetase DesD



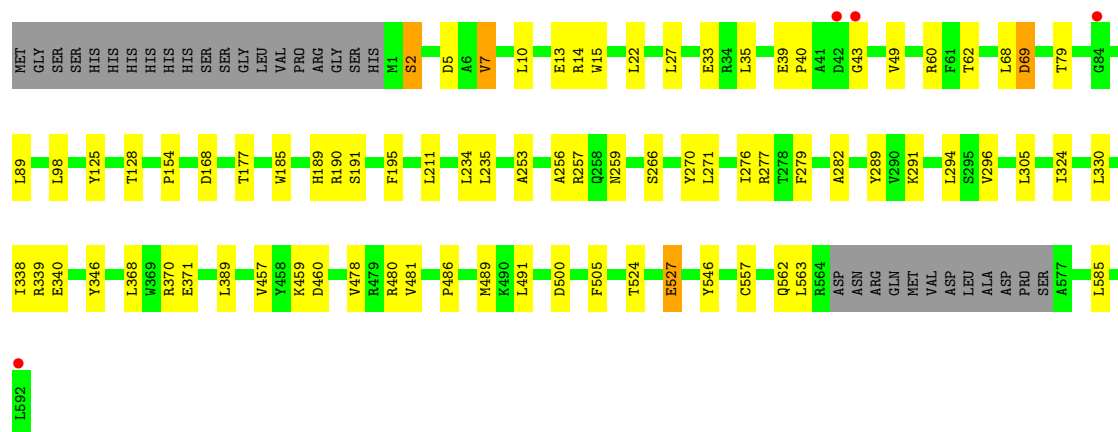
#### • Molecule 1: Desferrioxamine synthetase DesD



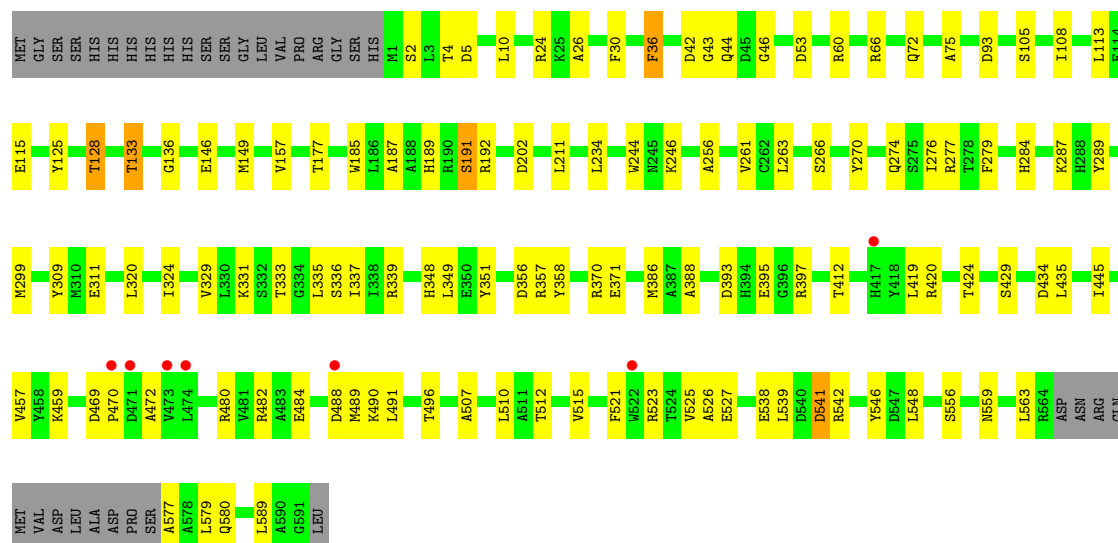
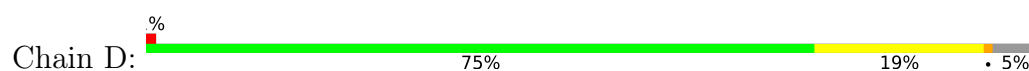
#### • Molecule 1: Desferrioxamine synthetase DesD



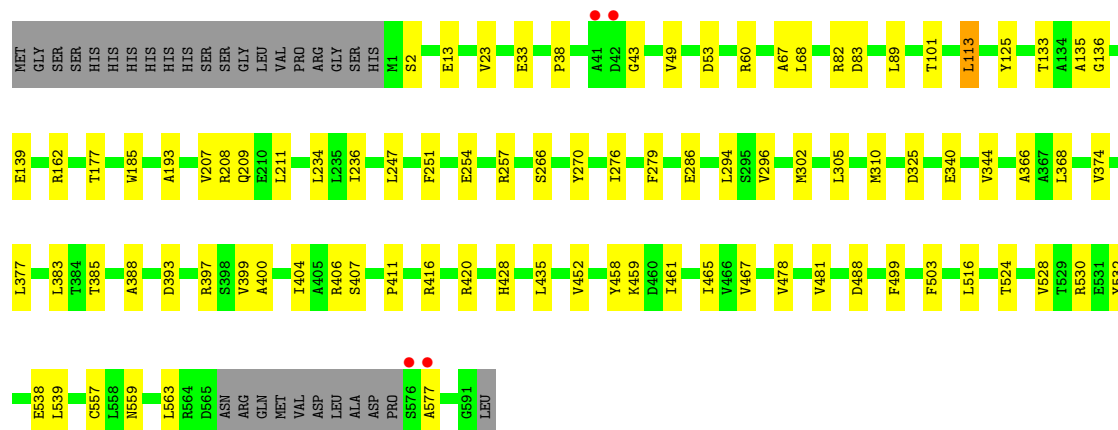
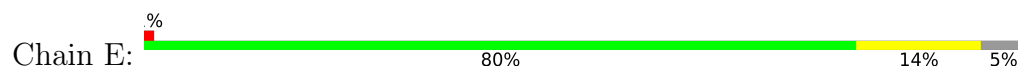




• Molecule 1: Desferrioxamine synthetase DesD



• 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, $\alpha$ , $\beta$ , $\gamma$	125.10Å 238.49Å 327.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.97 – 2.85 91.79 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (81.97-2.85) 93.6 (91.79-2.85)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.182 , 0.221 0.183 , 0.222	Depositor DCC
$R_{free}$ test set	5404 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.49	0/4670	0.69	0/6361
1	B	0.51	0/4677	0.70	2/6371 (0.0%)
1	C	0.46	0/4650	0.65	0/6335
1	D	0.46	0/4615	0.65	0/6297
1	E	0.44	0/4624	0.63	0/6307
All	All	0.47	0/23236	0.66	2/31671 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	289	TYR	CA-CB-CG	5.50	123.86	113.40

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	4558	0	4426	54	0
1	B	4561	0	4433	51	0
1	C	4538	0	4394	52	0
1	D	4499	0	4337	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4512	0	4356	45	0
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	0	0
4	D	14	0	0	2	0
4	E	12	0	0	0	0
All	All	22979	0	22058	257	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 (257) 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:E:133:THR:HB	1:E:136:GLY:H	1.45	0.81
1:D:489:MET:HE1	1:D:577:ALA:N	1.97	0.78
1:A:470:PRO:HG3	1:A:484:GLU:HG2	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:D:189:HIS:ND1	1:D:191:SER:HB3	2.05	0.70
1:D:115:GLU:HG3	1:D:299:MET:HE2	1.74	0.68
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
1:C:195:PHE:HB2	1:C:234:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:C:270:TYR:HB3	1:C:279:PHE:HB3	1.86	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:489:MET:HE3	1:B:576:SER:HB2	1.90	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:E:393:ASP:HB2	1:E:397:ARG:O	2.09	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
1:D:115:GLU:HG3	1:D:299:MET:CE	2.39	0.51
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:ASN:O	1:E:563:LEU:HG	2.11	0.50
1:E:13:GLU:CD	1:E:13:GLU:H	2.15	0.49
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:A:486:PRO:HG2	1:A:489:MET:CE	2.43	0.49
1:C:13:GLU:CD	1:C:13:GLU:H	2.16	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: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:B:13:GLU:CD	1:B:13:GLU:H	2.17	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
1:D:24:ARG:HD3	1:D:75:ALA:HB2	1.97	0.47
1:D:386:MET:HE2	1:D:386:MET:HB2	1.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:D:489:MET:HE3	1:D:489:MET:HB3	1.78	0.43
1:E:428:HIS:HA	1:E:532:TYR:OH	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:486:PRO:HG2	1:C:489:MET:CE	2.50	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:487:GLU:OE2	1:B:546:TYR:OH	2.27	0.42
1:E:302:MET:HB2	1:E:302:MET:HE2	1.72	0.42
1:E:305:LEU:HD22	1:E:310:MET:CE	2.50	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: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:A:486:PRO:HG2	1:A:489:MET:HE1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:214:GLU:H	1:A:214:GLU:CD	2.25	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

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%)	29	57
1	B	577/612 (94%)	546 (95%)	29 (5%)	2 (0%)	41	68
1	C	576/612 (94%)	546 (95%)	27 (5%)	3 (0%)	29	57
1	D	576/612 (94%)	550 (96%)	21 (4%)	5 (1%)	17	43
1	E	577/612 (94%)	548 (95%)	25 (4%)	4 (1%)	22	50
All	All	2882/3060 (94%)	2742 (95%)	123 (4%)	17 (1%)	25	53

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	ASP
1	A	43	GLY
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%)	454 (98%)	11 (2%)	49	77
1	B	467/504 (93%)	450 (96%)	17 (4%)	35	66
1	C	461/504 (92%)	452 (98%)	9 (2%)	55	80
1	D	454/504 (90%)	436 (96%)	18 (4%)	31	62
1	E	454/504 (90%)	443 (98%)	11 (2%)	49	77
All	All	2301/2520 (91%)	2235 (97%)	66 (3%)	42	72

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	47	ARG
1	A	69	ASP
1	A	89	LEU
1	A	130	PRO
1	A	207	VAL
1	A	331	LYS
1	A	379	ASP
1	A	385	THR
1	A	390	VAL
1	A	449	LYS
1	B	36	PHE
1	B	37	THR
1	B	45	ASP
1	B	79	THR
1	B	81	THR
1	B	82	ARG
1	B	128	THR
1	B	196	THR
1	B	214	GLU
1	B	309	TYR
1	B	383	LEU
1	B	385	THR

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Mol	Chain	Res	Type
1	B	416	ARG
1	B	434	ASP
1	B	440	HIS
1	B	493	SER
1	B	576	SER
1	C	7	VAL
1	C	40	PRO
1	C	62	THR
1	C	69	ASP
1	C	79	THR
1	C	89	LEU
1	C	98	LEU
1	C	389	LEU
1	C	527	GLU
1	D	36	PHE
1	D	93	ASP
1	D	128	THR
1	D	133	THR
1	D	191	SER
1	D	202	ASP
1	D	234	LEU
1	D	277	ARG
1	D	311	GLU
1	D	331	LYS
1	D	357	ARG
1	D	397	ARG
1	D	412	THR
1	D	459	LYS
1	D	482	ARG
1	D	488	ASP
1	D	490	LYS
1	D	541	ASP
1	E	2	SER
1	E	82	ARG
1	E	83	ASP
1	E	113	LEU
1	E	162	ARG
1	E	208	ARG
1	E	209	GLN
1	E	325	ASP
1	E	385	THR
1	E	459	LYS

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Mol	Chain	Res	Type
1	E	488	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	545	GLN
1	B	131	GLN
1	B	143	GLN
1	B	273	GLN
1	D	417	HIS
1	D	533	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	B	601	-	5,5,5	1.56	2 (40%)	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	604	-	4,4,4	0.81	0	6,6,6	0.29	0
2	GOL	B	603	-	5,5,5	1.12	0	5,5,5	1.15	0
3	SO4	A	609	-	4,4,4	0.33	0	6,6,6	0.37	0
3	SO4	A	611	-	4,4,4	0.85	0	6,6,6	0.22	0
3	SO4	B	606	-	4,4,4	0.55	0	6,6,6	0.44	0
3	SO4	C	610	-	4,4,4	0.68	0	6,6,6	0.66	0
2	GOL	E	601	-	5,5,5	1.58	1 (20%)	5,5,5	1.19	0
3	SO4	B	604	-	4,4,4	0.65	0	6,6,6	0.24	0
3	SO4	B	608	-	4,4,4	0.82	0	6,6,6	0.35	0
3	SO4	C	607	-	4,4,4	0.61	0	6,6,6	0.33	0
2	GOL	A	601	-	5,5,5	1.17	0	5,5,5	0.97	0
3	SO4	D	605	-	4,4,4	0.47	0	6,6,6	0.52	0
3	SO4	B	609	-	4,4,4	0.47	0	6,6,6	0.34	0
3	SO4	B	605	-	4,4,4	0.78	0	6,6,6	0.35	0
2	GOL	D	601	-	5,5,5	1.82	2 (40%)	5,5,5	0.88	0
3	SO4	A	607	-	4,4,4	0.65	0	6,6,6	0.31	0
3	SO4	D	603	-	4,4,4	0.62	0	6,6,6	0.33	0
2	GOL	C	605	-	5,5,5	1.18	0	5,5,5	0.88	0
2	GOL	A	603	-	5,5,5	0.93	0	5,5,5	0.91	0
3	SO4	A	605	-	4,4,4	0.63	0	6,6,6	0.41	0
3	SO4	C	611	-	4,4,4	0.77	0	6,6,6	0.26	0
3	SO4	D	606	-	4,4,4	0.72	0	6,6,6	0.32	0
3	SO4	E	602	-	4,4,4	0.58	0	6,6,6	0.50	0
3	SO4	C	608	-	4,4,4	0.36	0	6,6,6	0.35	0
3	SO4	E	603	-	4,4,4	0.47	0	6,6,6	0.30	0
2	GOL	C	602	-	5,5,5	1.33	1 (20%)	5,5,5	1.21	0
2	GOL	C	601	-	5,5,5	1.07	0	5,5,5	0.86	0
2	GOL	B	602	-	5,5,5	1.22	1 (20%)	5,5,5	1.27	1 (20%)
3	SO4	E	604	-	4,4,4	0.78	0	6,6,6	0.32	0
2	GOL	C	604	-	5,5,5	1.06	0	5,5,5	1.45	1 (20%)
2	GOL	D	602	-	5,5,5	1.93	2 (40%)	5,5,5	0.75	0
3	SO4	C	606	-	4,4,4	0.65	0	6,6,6	0.52	0
3	SO4	C	609	-	4,4,4	0.80	0	6,6,6	0.41	0
3	SO4	B	607	-	4,4,4	0.37	0	6,6,6	0.70	0
3	SO4	A	608	-	4,4,4	0.75	0	6,6,6	0.29	0
3	SO4	A	604	-	4,4,4	0.45	0	6,6,6	0.34	0
3	SO4	A	606	-	4,4,4	0.65	0	6,6,6	0.47	0
2	GOL	C	603	-	5,5,5	0.92	0	5,5,5	0.86	0
3	SO4	A	610	-	4,4,4	0.72	0	6,6,6	0.44	0
2	GOL	A	602	-	5,5,5	1.07	1 (20%)	5,5,5	0.91	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	B	601	-	-	4/4/4/4	-
2	GOL	E	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	C	604	-	-	4/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	C	601	-	-	1/4/4/4	-
2	GOL	B	603	-	-	1/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	GOL	C1-C2	3.33	1.65	1.51
2	D	601	GOL	C1-C2	3.17	1.64	1.51
2	E	601	GOL	C1-C2	3.13	1.64	1.51
2	B	601	GOL	C1-C2	2.59	1.62	1.51
2	C	602	GOL	C3-C2	2.56	1.62	1.51
2	D	602	GOL	C3-C2	2.43	1.61	1.51
2	D	601	GOL	C3-C2	2.32	1.61	1.51
2	B	602	GOL	C3-C2	2.29	1.61	1.51
2	B	601	GOL	C3-C2	2.17	1.60	1.51
2	A	602	GOL	C1-C2	2.02	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	GOL	C3-C2-C1	-2.21	103.12	111.70
2	C	604	GOL	C3-C2-C1	-2.12	103.48	111.70

There are no chirality outliers.



All (22) 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	C	604	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	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	B	603	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-O2
2	C	604	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 12 short contacts:

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

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	580/612 (94%)	-0.02	2 (0%) 94 94	26, 45, 73, 116	0
1	B	580/612 (94%)	-0.14	1 (0%) 95 95	26, 43, 73, 104	0
1	C	580/612 (94%)	0.01	4 (0%) 87 87	35, 50, 75, 112	0
1	D	579/612 (94%)	0.08	7 (1%) 79 78	34, 54, 84, 119	0
1	E	581/612 (94%)	0.05	4 (0%) 87 87	37, 57, 81, 120	0
All	All	2900/3060 (94%)	-0.01	18 (0%) 89 89	26, 50, 78, 120	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	42	ASP	4.6
1	E	42	ASP	3.1
1	C	43	GLY	3.1
1	C	592	LEU	3.0
1	D	471	ASP	3.0
1	D	473	VAL	2.7
1	D	470	PRO	2.7
1	D	474	LEU	2.5
1	B	576	SER	2.5
1	D	417	HIS	2.3
1	E	576	SER	2.3
1	E	41	ALA	2.3
1	D	522	TRP	2.3
1	D	488	ASP	2.2
1	A	41	ALA	2.2
1	E	577	ALA	2.1
1	A	43	GLY	2.1
1	C	84	GLY	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 monosaccharides 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, 95<sup>th</sup> 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	D	601	6/6	0.78	0.23	51,57,58,58	0
2	GOL	B	603	6/6	0.79	0.33	58,62,64,65	0
2	GOL	C	602	6/6	0.83	0.23	53,60,62,65	0
2	GOL	E	601	6/6	0.83	0.28	46,48,55,60	0
2	GOL	B	602	6/6	0.84	0.35	47,48,51,53	0
2	GOL	C	601	6/6	0.85	0.23	75,81,81,85	0
2	GOL	A	601	6/6	0.85	0.32	65,69,74,79	0
2	GOL	C	604	6/6	0.87	0.20	57,61,66,66	0
3	SO4	B	605	5/5	0.87	0.26	65,65,69,80	0
2	GOL	A	603	6/6	0.88	0.22	72,75,75,76	0
2	GOL	D	602	6/6	0.88	0.26	45,47,48,51	0
3	SO4	A	608	5/5	0.89	0.39	58,64,77,79	0
3	SO4	D	604	5/5	0.91	0.24	62,64,67,79	0
3	SO4	A	611	5/5	0.92	0.39	64,65,76,79	0
3	SO4	B	604	5/5	0.92	0.31	60,61,76,77	0
3	SO4	A	607	5/5	0.92	0.31	68,73,78,82	0
3	SO4	C	609	5/5	0.92	0.34	65,65,75,77	0
2	GOL	B	601	6/6	0.92	0.21	41,43,47,49	0
3	SO4	E	604	5/5	0.92	0.29	72,74,84,88	0
3	SO4	C	610	5/5	0.93	0.16	62,62,67,72	0
3	SO4	C	606	5/5	0.93	0.37	68,75,77,82	0
3	SO4	E	602	5/5	0.93	0.20	55,57,66,67	0
3	SO4	B	608	5/5	0.93	0.20	65,66,73,81	0
3	SO4	D	603	5/5	0.94	0.21	65,66,76,79	0
3	SO4	A	610	5/5	0.94	0.29	59,64,74,76	0
2	GOL	C	605	6/6	0.94	0.50	58,59,65,65	0
3	SO4	C	611	5/5	0.94	0.18	66,69,75,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	603	6/6	0.95	0.22	56,58,59,62	0
3	SO4	A	605	5/5	0.95	0.23	61,63,78,78	0
3	SO4	A	606	5/5	0.95	0.17	52,54,63,65	0
3	SO4	D	605	5/5	0.96	0.15	60,61,68,69	0
2	GOL	A	602	6/6	0.96	0.12	38,39,41,46	0
3	SO4	E	603	5/5	0.96	0.15	59,60,64,65	0
3	SO4	B	609	5/5	0.96	0.22	62,64,68,70	0
3	SO4	B	607	5/5	0.97	0.17	45,49,53,54	0
3	SO4	C	607	5/5	0.97	0.19	55,56,67,70	0
3	SO4	D	606	5/5	0.97	0.29	73,74,77,84	0
3	SO4	A	609	5/5	0.98	0.18	50,51,55,56	0
3	SO4	C	608	5/5	0.98	0.14	54,54,60,60	0
3	SO4	B	606	5/5	0.98	0.10	49,51,63,64	0
3	SO4	A	604	5/5	0.98	0.13	54,55,57,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.