



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GOY  
Title : The crystal structure of human fascin 1 K41A mutant  
Authors : Yang, S.Y.; Huang, F.K.; Huang, J.; Chen, S.; Jakoncic, J.; Leo-Macias, A.;  
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Deposited on : 2012-08-20  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

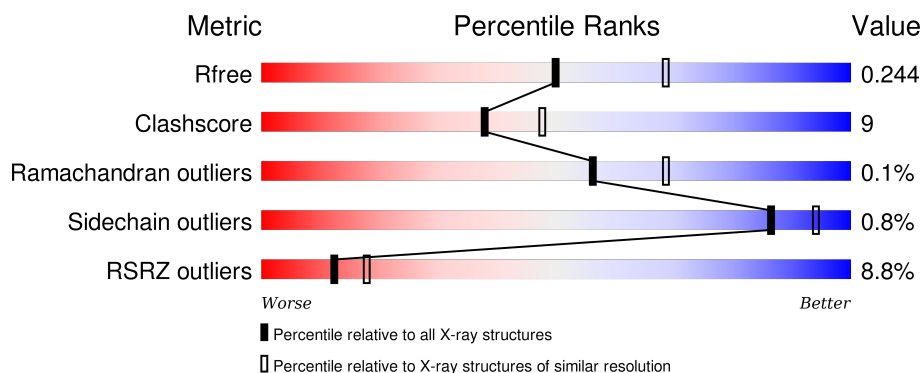
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	493	<div> <div>9%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	B	493	<div> <div>8%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>

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	BR	A	501	-	-	X	-
2	BR	B	504	-	-	X	-
4	GOL	B	513	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8000 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 Fascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	1	0
			3701	2317	656	713	15			
1	B	484	Total	C	N	O	S	0	3	0
			3786	2367	676	726	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	LYS	ENGINEERED MUTATION	UNP Q16658
B	41	ALA	LYS	ENGINEERED MUTATION	UNP Q16658

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Br	0	0
			5	5		
2	A	3	Total	Br	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

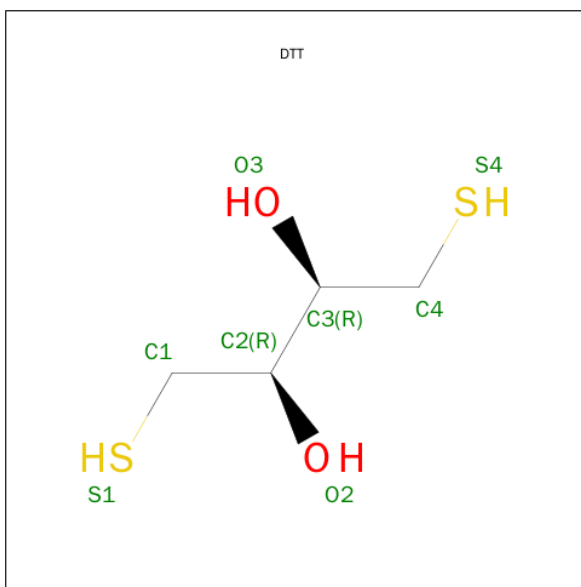
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total	Cl	0	0
			6	6		
3	A	4	Total	Cl	0	0
			4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			8	4	2	2		

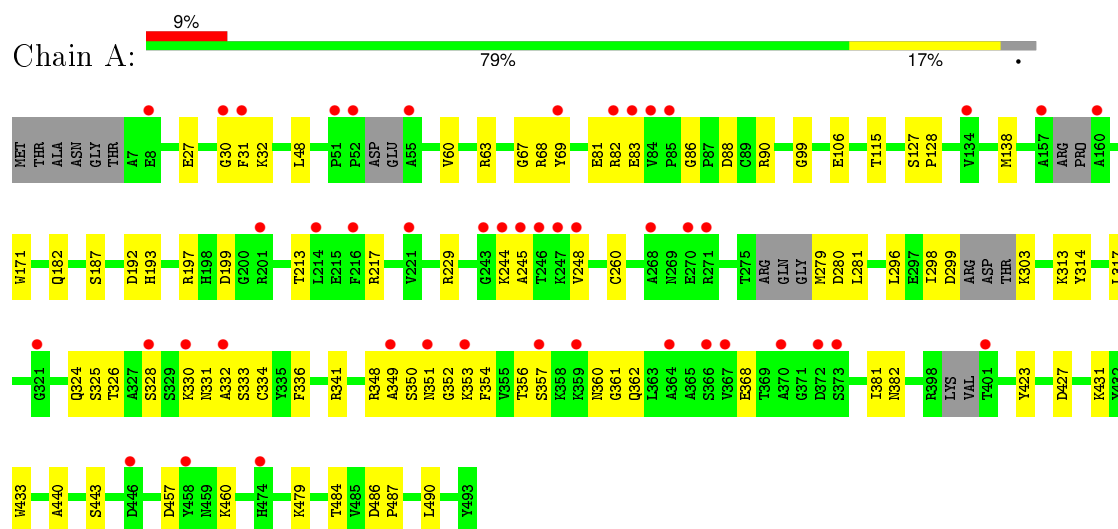
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total	O	0	0
			222	222		
6	B	229	Total	O	0	0
			229	229		

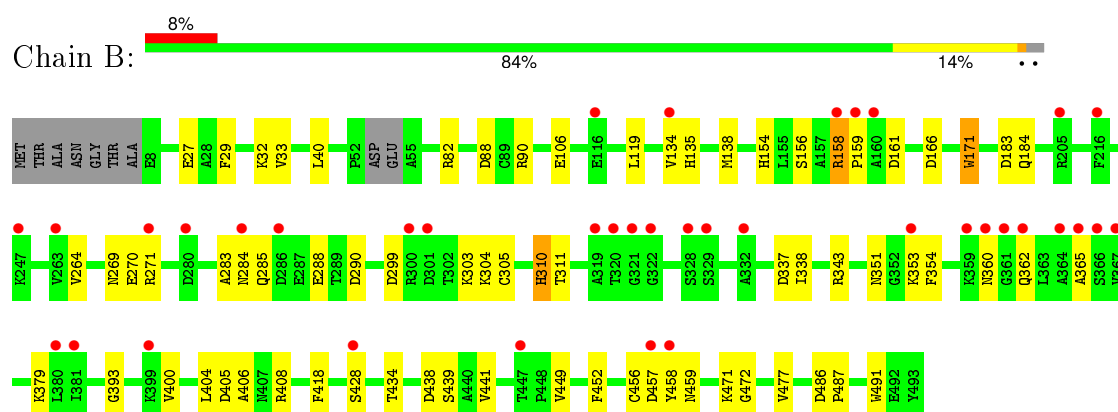
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Fascin



#### • Molecule 1: Fascin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.14Å 70.59Å 110.98Å 90.00° 130.63° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 28.35 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.30) 98.9 (28.35-2.29)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.245 0.201 , 0.244	Depositor DCC
$R_{free}$ test set	2123 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.1	EDS
Estimated twinning fraction	0.025 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42272 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, BR, DTT

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	0.55	1/3779 (0.0%)	0.66	0/5105
1	B	0.54	1/3875 (0.0%)	0.66	0/5239
All	All	0.55	2/7654 (0.0%)	0.66	0/10344

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	TRP	CD2-CE2	5.32	1.47	1.41
1	B	171	TRP	CD2-CE2	5.06	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	LYS	Peptide
1	B	456	CYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3701	0	3574	83	0
1	B	3786	0	3673	54	0
2	A	3	0	0	2	0
2	B	5	0	0	3	0
3	A	4	0	0	0	0
3	B	6	0	0	0	0
4	A	18	0	24	3	0
4	B	18	0	24	2	0
5	B	8	0	10	1	0
6	A	222	0	0	12	0
6	B	229	0	0	4	0
All	All	8000	0	7305	136	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 9.

All (136) 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:360:ASN:HD22	1:B:362:GLN:NE2	1.51	1.09
1:B:360:ASN:ND2	1:B:362:GLN:HE21	1.56	1.03
1:A:48:LEU:HD11	1:A:60:VAL:HB	1.41	0.99
1:B:29:PHE:HB2	5:B:515:DTT:H42	1.52	0.90
1:A:68:ARG:NH1	1:A:81:GLU:O	2.06	0.87
1:A:348:ARG:CD	6:A:783:HOH:O	2.22	0.86
1:A:299:ASP:HB2	1:A:303:LYS:N	1.92	0.85
1:A:341:ARG:HH11	1:A:341:ARG:HG2	1.47	0.79
1:A:30:GLY:O	1:A:32:LYS:HG3	1.81	0.79
1:A:48:LEU:HD11	1:A:60:VAL:CB	2.12	0.79
1:A:324:GLN:HG3	1:A:326:THR:OG1	1.88	0.73
1:A:182:GLN:NE2	1:A:187:SER:OG	2.21	0.73
1:B:82:ARG:HD3	2:B:504:BR:BR	2.44	0.72
1:A:348:ARG:CG	6:A:783:HOH:O	2.38	0.72
1:A:30:GLY:C	1:A:32:LYS:HG3	2.10	0.71
1:B:290:ASP:HB3	1:B:310:HIS:ND1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LYS:HE2	1:A:368:GLU:HG2	1.73	0.70
1:A:486:ASP:HB2	1:A:487:PRO:CD	2.21	0.70
1:A:348:ARG:HD3	6:A:783:HOH:O	1.86	0.70
1:A:356:THR:HG22	1:A:357:SER:N	2.07	0.70
1:A:349:ALA:O	1:A:352:GLY:N	2.13	0.67
1:B:351:ASN:HB3	1:B:353:LYS:H	1.59	0.67
1:A:299:ASP:CB	1:A:303:LYS:N	2.56	0.67
1:A:68:ARG:CZ	1:A:83:GLU:HG3	2.25	0.67
1:B:459:ASN:N	1:B:459:ASN:OD1	2.29	0.66
1:A:353:LYS:HE2	1:A:368:GLU:CG	2.26	0.66
1:B:393:GLY:HA2	4:B:513:GOL:H12	1.79	0.65
1:A:486:ASP:HB2	1:A:487:PRO:HD3	1.78	0.65
1:A:48:LEU:CD1	1:A:60:VAL:HB	2.23	0.64
1:A:115:THR:HB	6:A:668:HOH:O	1.97	0.64
1:B:284:ASN:OD1	1:B:285:GLN:HG2	1.98	0.63
1:B:158:ARG:H	1:B:159:PRO:CD	2.11	0.63
1:B:158:ARG:H	1:B:159:PRO:HD2	1.63	0.62
1:A:82:ARG:HG2	6:A:767:HOH:O	1.98	0.62
1:A:30:GLY:CA	1:A:32:LYS:HE2	2.30	0.62
1:A:423:TYR:HE2	4:A:508:GOL:H31	1.65	0.62
1:A:431:LYS:HE2	1:A:443:SER:O	2.00	0.61
1:A:314:TYR:CZ	1:A:330:LYS:HE2	2.35	0.61
1:A:341:ARG:HG2	1:A:341:ARG:NH1	2.11	0.61
1:A:99:GLY:HA2	1:A:213:THR:OG1	2.00	0.61
1:B:360:ASN:HB2	1:B:362:GLN:HG2	1.82	0.60
1:A:331:ASN:HB2	6:A:624:HOH:O	2.01	0.60
1:A:317:LEU:HB3	1:A:333:SER:HB3	1.83	0.60
1:A:348:ARG:HG3	6:A:783:HOH:O	1.99	0.60
1:A:127:SER:HB2	1:A:128:PRO:HD2	1.84	0.59
1:A:354:PHE:CG	6:A:783:HOH:O	2.52	0.59
1:B:82:ARG:CD	2:B:504:BR:BR	3.05	0.59
1:A:63:ARG:HE	1:A:67:GLY:HA2	1.67	0.59
1:B:351:ASN:ND2	1:B:353:LYS:HD3	2.18	0.58
1:B:458:TYR:HB3	1:B:459:ASN:OD1	2.04	0.58
1:B:158:ARG:HB2	1:B:159:PRO:HD3	1.86	0.57
1:A:360:ASN:C	1:A:360:ASN:OD1	2.42	0.57
1:B:310:HIS:CD2	1:B:311:THR:HG23	2.39	0.57
1:A:440:ALA:HA	1:A:479:LYS:HG2	1.86	0.57
1:B:487:PRO:HD3	6:B:803:HOH:O	2.02	0.57
1:B:134:VAL:HG11	6:B:766:HOH:O	2.05	0.57
1:A:332:ALA:O	1:A:350:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:OE1	1:A:32:LYS:HB2	2.06	0.56
1:A:217:ARG:NH1	1:A:248:VAL:HB	2.20	0.56
1:B:406:ALA:HB1	1:B:491:TRP:HH2	1.71	0.56
1:A:88:ASP:HB2	2:A:501:BR:BR	2.60	0.56
1:A:484:THR:HG21	1:B:477:VAL:CG2	2.37	0.55
1:A:30:GLY:HA3	1:A:32:LYS:HE2	1.87	0.55
1:B:264:VAL:HG21	1:B:288:GLU:HG2	1.89	0.54
1:B:158:ARG:N	1:B:159:PRO:CD	2.70	0.54
1:A:351:ASN:OD1	1:A:353:LYS:HB2	2.08	0.54
1:A:331:ASN:H	1:A:334:CYS:HB2	1.72	0.54
1:A:353:LYS:CE	1:A:368:GLU:HG2	2.37	0.54
1:A:229:ARG:HA	1:A:245:ALA:O	2.08	0.54
1:A:279:MET:HE1	1:A:313:LYS:HG3	1.91	0.53
1:A:317:LEU:CD2	1:A:351:ASN:HB2	2.38	0.53
1:A:281:LEU:HD21	1:A:325:SER:HB3	1.90	0.52
1:A:328:SER:H	4:A:510:GOL:H32	1.74	0.52
1:B:269:ASN:HD21	1:B:283:ALA:HB3	1.74	0.52
1:A:68:ARG:CZ	1:A:83:GLU:CG	2.87	0.52
1:A:457:ASP:HB3	1:A:460:LYS:HB2	1.92	0.52
1:B:183:ASP:O	1:B:184:GLN:CB	2.56	0.52
1:A:86:GLY:HA3	2:A:501:BR:BR	2.64	0.52
1:A:260[B]:CYS:SG	1:A:296:LEU:O	2.68	0.51
1:A:317:LEU:HD21	1:A:351:ASN:HB2	1.92	0.50
1:B:27:GLU:HB2	1:B:32:LYS:HB2	1.94	0.50
1:A:490:LEU:HD13	1:B:400:VAL:HG11	1.94	0.50
1:B:360:ASN:ND2	1:B:362:GLN:NE2	2.32	0.49
1:A:354:PHE:N	6:A:783:HOH:O	2.45	0.49
1:A:68:ARG:NH1	1:A:83:GLU:HG3	2.27	0.49
1:B:354:PHE:O	1:B:365:ALA:HA	2.12	0.49
1:B:88:ASP:HB2	2:B:501:BR:BR	2.69	0.48
1:B:304:LYS:NZ	1:B:337:ASP:OD1	2.38	0.48
1:B:360:ASN:HD22	1:B:362:GLN:HE21	0.71	0.48
1:B:271:ARG:HD3	1:B:284:ASN:HA	1.96	0.48
1:A:63:ARG:HD2	1:A:69:TYR:CZ	2.49	0.47
1:A:63:ARG:NE	1:A:67:GLY:HA2	2.30	0.47
1:A:354:PHE:CD1	6:A:783:HOH:O	2.67	0.47
1:A:356:THR:CG2	1:A:357:SER:N	2.74	0.47
1:B:404:LEU:HD12	1:B:441:VAL:HG12	1.97	0.47
1:B:90:ARG:HD3	1:B:106:GLU:OE1	2.15	0.47
1:A:330:LYS:HE3	6:A:762:HOH:O	2.15	0.47
1:A:427:ASP:OD1	1:A:431:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLY:HA3	1:A:32:LYS:CE	2.46	0.46
1:A:336:PHE:CE1	1:A:349:ALA:HB2	2.50	0.46
1:B:183:ASP:O	1:B:184:GLN:HB3	2.16	0.46
1:B:299:ASP:O	1:B:303:LYS:N	2.46	0.45
1:A:423:TYR:HE2	4:A:508:GOL:C3	2.28	0.45
1:B:310:HIS:HD2	1:B:311:THR:HG23	1.81	0.45
1:A:333:SER:HB2	6:A:624:HOH:O	2.17	0.44
1:A:298:ILE:O	1:A:299:ASP:C	2.54	0.44
1:B:303:LYS:HG2	6:B:772:HOH:O	2.17	0.44
1:B:486:ASP:HB2	1:B:487:PRO:HD2	2.00	0.44
1:A:361:GLY:O	1:A:362:GLN:C	2.55	0.44
1:A:90:ARG:HD3	1:A:106:GLU:OE1	2.17	0.44
1:A:68:ARG:HD2	1:A:81:GLU:O	2.17	0.44
1:B:343:ARG:HG2	1:B:452:PHE:HE1	1.83	0.44
1:B:379:LYS:HD3	1:B:418:PHE:CD2	2.52	0.44
1:A:31:PHE:CD1	1:A:81:GLU:HG3	2.53	0.43
1:B:154:HIS:NE2	1:B:166:ASP:OD1	2.48	0.43
1:A:353:LYS:CD	1:A:368:GLU:HG2	2.49	0.43
1:A:280:ASP:OD2	1:A:280:ASP:N	2.48	0.43
1:A:331:ASN:O	1:A:334:CYS:HB2	2.19	0.43
1:A:486:ASP:CB	1:A:487:PRO:CD	2.95	0.43
1:B:269:ASN:O	1:B:270:GLU:HB2	2.19	0.42
1:B:305[B]:CYS:SG	1:B:338:ILE:HD11	2.58	0.42
1:A:381:ILE:HD12	1:A:382:ASN:N	2.34	0.42
1:B:471:LYS:HD3	1:B:472:GLY:O	2.18	0.42
1:B:434:THR:HG22	1:B:449:VAL:HG23	2.02	0.42
1:B:438:ASP:O	1:B:439:SER:HB2	2.19	0.42
1:A:360:ASN:OD1	1:A:360:ASN:O	2.38	0.42
1:B:405:ASP:HB2	1:B:408:ARG:HD3	2.02	0.41
1:B:158:ARG:N	1:B:159:PRO:HD2	2.31	0.41
1:A:30:GLY:HA3	1:A:32:LYS:CD	2.51	0.41
1:B:457:ASP:OD1	1:B:458:TYR:N	2.54	0.41
1:A:192:ASP:O	1:A:193:HIS:HB2	2.21	0.41
1:B:40:LEU:HD22	1:B:135:HIS:CG	2.56	0.41
1:B:33:VAL:HG12	1:B:119:LEU:HD12	2.03	0.41
4:B:513:GOL:H11	6:B:679:HOH:O	2.19	0.40
1:A:197:ARG:NH1	1:A:199:ASP:OD2	2.53	0.40
1:B:156:SER:O	1:B:161:ASP:OD1	2.38	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	464/493 (94%)	440 (95%)	24 (5%)	0	100	100
1	B	483/493 (98%)	458 (95%)	24 (5%)	1 (0%)	52	64
All	All	947/986 (96%)	898 (95%)	48 (5%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	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	389/403 (96%)	387 (100%)	2 (0%)	92	97
1	B	400/403 (99%)	396 (99%)	4 (1%)	82	91
All	All	789/806 (98%)	783 (99%)	6 (1%)	86	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	A	171	TRP
1	B	138	MET
1	B	171	TRP
1	B	310	HIS

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Mol	Chain	Res	Type
1	B	428	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	182	GLN
1	A	193	HIS
1	A	198	HIS
1	B	362	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 18 are monoatomic - leaving 7 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	GOL	A	508	-	5,5,5	0.20	0	5,5,5	0.39	0
4	GOL	A	509	-	5,5,5	0.26	0	5,5,5	0.69	0
4	GOL	A	510	-	5,5,5	0.21	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	512	-	5,5,5	0.24	0	5,5,5	0.45	0
4	GOL	B	513	-	5,5,5	0.27	0	5,5,5	0.32	0
4	GOL	B	514	-	5,5,5	0.15	0	5,5,5	0.37	0
5	DTT	B	515	-	7,7,7	0.54	0	4,8,8	1.91	2 (50%)

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
4	GOL	A	508	-	-	0/4/4/4	0/0/0/0
4	GOL	A	509	-	-	0/4/4/4	0/0/0/0
4	GOL	A	510	-	-	0/4/4/4	0/0/0/0
4	GOL	B	512	-	-	0/4/4/4	0/0/0/0
4	GOL	B	513	-	-	0/4/4/4	0/0/0/0
4	GOL	B	514	-	-	0/4/4/4	0/0/0/0
5	DTT	B	515	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	515	DTT	C2-C1-S1	-2.75	109.34	113.91
5	B	515	DTT	C3-C4-S4	-2.66	109.51	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	508	GOL	2	0
4	A	510	GOL	1	0
4	B	513	GOL	2	0
5	B	515	DTT	1	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	475/493 (96%)	0.51	46 (9%) 10 14	19, 36, 67, 89	0
1	B	484/493 (98%)	0.44	38 (7%) 15 22	16, 34, 65, 90	0
All	All	959/986 (97%)	0.47	84 (8%) 12 18	16, 35, 67, 90	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	ASP	6.3
1	A	244	LYS	6.3
1	B	458	TYR	5.9
1	B	158	ARG	5.6
1	A	359	LYS	5.4
1	A	246	THR	5.0
1	A	373	SER	4.7
1	A	401	THR	4.4
1	A	247	LYS	4.4
1	A	160	ALA	4.4
1	B	159	PRO	4.2
1	B	360	ASN	4.2
1	B	366	SER	4.1
1	A	332	ALA	4.1
1	B	447	THR	4.0
1	A	364	ALA	4.0
1	A	367	VAL	3.9
1	B	367	VAL	3.8
1	A	474	HIS	3.7
1	B	321	GLY	3.7
1	B	320	THR	3.3
1	A	458	TYR	3.3
1	A	321	GLY	3.3
1	B	361	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	ALA	3.2
1	A	268	ALA	3.2
1	B	359	LYS	3.2
1	A	248	VAL	3.1
1	B	300	ARG	3.1
1	A	216	PHE	3.1
1	B	381	ILE	3.1
1	B	301	ASP	3.0
1	A	31	PHE	3.0
1	A	84	VAL	3.0
1	B	116	GLU	3.0
1	A	351	ASN	2.9
1	A	245	ALA	2.9
1	B	399	LYS	2.9
1	B	365	ALA	2.8
1	A	52	PRO	2.8
1	B	263	VAL	2.8
1	A	134	VAL	2.8
1	A	82	ARG	2.7
1	A	214	LEU	2.7
1	B	328	SER	2.7
1	B	286	ASP	2.7
1	B	160	ALA	2.6
1	B	247	LYS	2.6
1	A	446	ASP	2.6
1	B	271	ARG	2.6
1	A	243	GLY	2.5
1	A	55	ALA	2.5
1	B	428	SER	2.5
1	A	157	ALA	2.5
1	A	201	ARG	2.5
1	B	322	GLY	2.5
1	B	319	ALA	2.5
1	A	357	SER	2.4
1	B	329	SER	2.4
1	A	83	GLU	2.4
1	A	349	ALA	2.4
1	B	332	ALA	2.4
1	B	364	ALA	2.4
1	B	216	PHE	2.4
1	B	205	ARG	2.3
1	A	30	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	353	LYS	2.2
1	B	284	ASN	2.2
1	A	330	LYS	2.2
1	A	69	TYR	2.2
1	A	221	VAL	2.2
1	B	280	ASP	2.1
1	B	134	VAL	2.1
1	A	270	GLU	2.1
1	A	85	PRO	2.1
1	A	366	SER	2.1
1	B	380	LEU	2.1
1	A	271	ARG	2.1
1	A	328	SER	2.1
1	B	353	LYS	2.0
1	A	8	GLU	2.0
1	B	362	GLN	2.0
1	A	51	PRO	2.0
1	A	372	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	513	6/6	0.85	0.19	2.38	39,42,46,47	0
3	CL	B	511	1/1	0.93	0.22	1.57	48,48,48,48	0
5	DTT	B	515	8/8	0.78	0.25	1.52	61,66,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	512	6/6	0.90	0.28	1.48	28,32,35,38	0
4	GOL	A	508	6/6	0.92	0.16	1.17	30,38,40,42	0
3	CL	A	507	1/1	0.82	0.24	0.89	62,62,62,62	0
4	GOL	A	509	6/6	0.95	0.15	0.78	33,40,43,47	0
4	GOL	A	510	6/6	0.81	0.22	0.78	58,62,63,63	0
4	GOL	B	514	6/6	0.90	0.15	0.09	35,39,41,44	0
3	CL	B	507	1/1	0.97	0.15	0.03	43,43,43,43	0
3	CL	B	506	1/1	0.98	0.11	-0.73	35,35,35,35	0
2	BR	A	501	1/1	0.98	0.06	-1.21	49,49,49,49	0
3	CL	B	508	1/1	0.93	0.07	-1.47	44,44,44,44	0
2	BR	A	503	1/1	0.98	0.05	-1.82	65,65,65,65	0
3	CL	A	504	1/1	0.96	0.11	-	48,48,48,48	0
2	BR	B	502	1/1	0.99	0.05	-	45,45,45,45	0
2	BR	A	502	1/1	0.97	0.05	-	49,49,49,49	0
3	CL	A	506	1/1	0.89	0.10	-	58,58,58,58	0
2	BR	B	504	1/1	0.94	0.11	-	65,65,65,65	0
3	CL	B	509	1/1	0.89	0.06	-	74,74,74,74	0
3	CL	B	510	1/1	0.96	0.05	-	63,63,63,63	0
2	BR	B	503	1/1	0.99	0.04	-	52,52,52,52	0
2	BR	B	501	1/1	0.99	0.04	-	41,41,41,41	0
3	CL	A	505	1/1	0.99	0.11	-	41,41,41,41	0
2	BR	B	505	1/1	0.97	0.03	-	66,66,66,66	0

## 6.5 Other polymers

There are no such residues in this entry.