



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:40 pm BST

PDB ID : 1BY3  
Title : FHUA FROM E. COLI  
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Deposited on : 1998-10-22  
Resolution : 2.74 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.

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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 : 2.11  
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) : 2.11

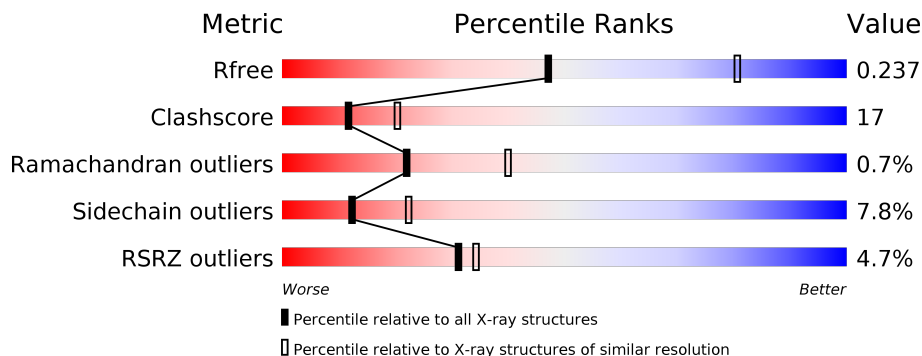
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

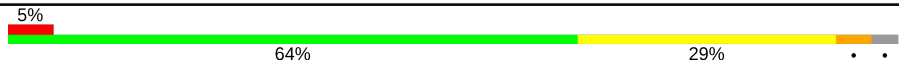
The reported resolution of this entry is 2.74 Å.

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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 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	714	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5677 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.

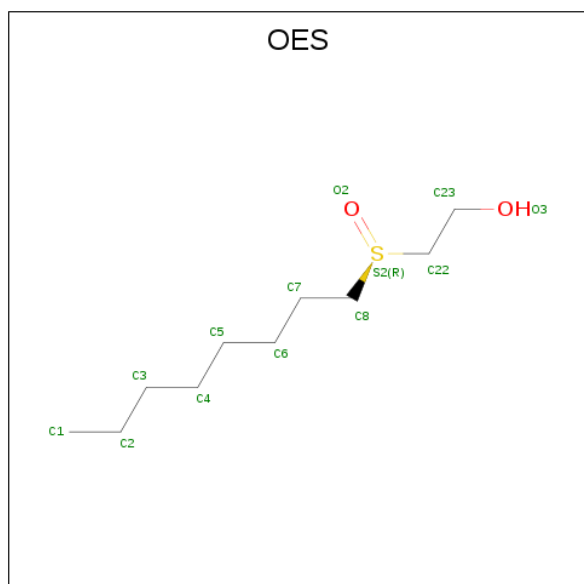
- Molecule 1 is a protein called PROTEIN (FERRICHROME-IRON RECEPTOR PRECURSOR (FHUA)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	695	5435	3425	923	1073	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	ARG	ALA	CONFLICT	UNP P06971
A	577	PRO	ALA	CONFLICT	UNP P06971

- Molecule 2 is N-OCTYL-2-HYDROXYETHYL SULFOXIDE (three-letter code: OES) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	13	10	2	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			13	10	2	1		
2	A	1	Total	C	O	S	0	0
			13	10	2	1		
2	A	1	Total	C	O	S	0	0
			13	10	2	1		
2	A	1	Total	C	O	S	0	0
			13	10	2	1		
2	A	1	Total	C	O	S	0	0
			13	10	2	1		

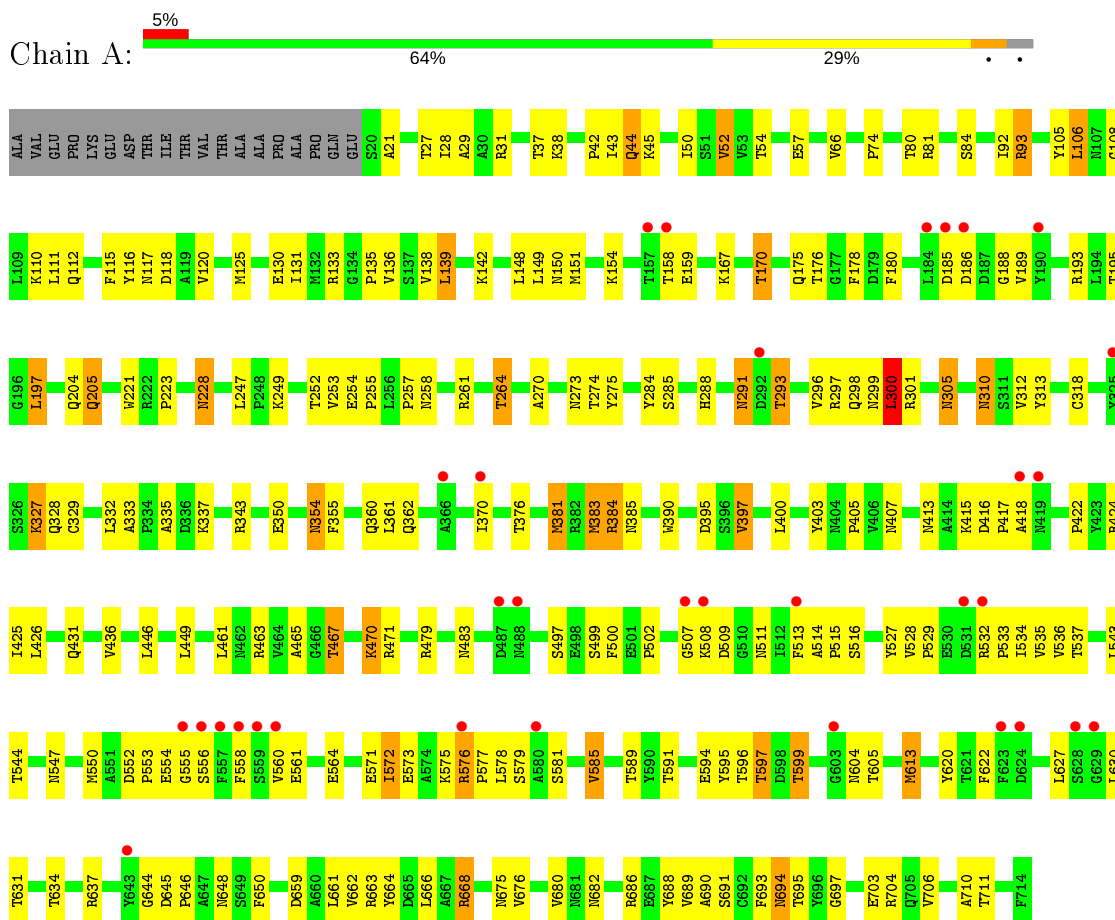
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total	O	0	0
			151	151		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: PROTEIN (FERRICHRROME-IRON RECEPTOR PRECURSOR (FHUA))



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.90Å 89.90Å 90.00Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	12.00 – 2.74 29.36 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.0 (12.00-2.74) 92.7 (29.36-2.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.76Å)	Xtrriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.186 , 0.244 0.188 , 0.237	Depositor DCC
$R_{free}$ test set	1333 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtrriage
Anisotropy	0.220	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OES

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	0.37	0/5570	0.63	2/7569 (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	A	300	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	310	ASN	N-CA-C	-5.04	97.40	111.00

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	5435	0	5162	189	0
2	A	91	0	154	5	0
3	A	151	0	0	11	0
All	All	5677	0	5316	189	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 17.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:HB3	1:A:597:THR:HG23	1.45	0.98
1:A:575:LYS:HG2	1:A:585:VAL:HG22	1.48	0.95
1:A:533:PRO:O	1:A:577:PRO:HD2	1.65	0.95
1:A:694:ASN:HD22	1:A:695:THR:H	1.15	0.93
1:A:135:PRO:HB3	1:A:499:SER:HB3	1.52	0.92
1:A:547:ASN:HD21	1:A:561:GLU:HB3	1.35	0.89
1:A:27:THR:HG21	1:A:577:PRO:HD3	1.57	0.87
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.58	0.84
1:A:664:TYR:OH	1:A:668:ARG:HG3	1.79	0.81
1:A:694:ASN:ND2	1:A:695:THR:H	1.80	0.80
1:A:328:GLN:HE21	1:A:395:ASP:HA	1.47	0.79
1:A:249:LYS:HB2	1:A:253:VAL:HG22	1.63	0.78
1:A:663:ARG:HD3	3:A:1040:HOH:O	1.82	0.78
1:A:264:THR:HG21	1:A:703:GLU:HG2	1.66	0.77
1:A:158:THR:HG22	1:A:159:GLU:OE2	1.86	0.74
1:A:694:ASN:HD22	1:A:695:THR:N	1.86	0.74
1:A:327:LYS:HE3	1:A:395:ASP:OD2	1.89	0.72
1:A:547:ASN:ND2	1:A:561:GLU:HB3	2.04	0.72
1:A:249:LYS:HB2	1:A:253:VAL:CG2	2.20	0.71
1:A:527:TYR:CD2	1:A:534:ILE:HD11	2.26	0.70
1:A:284:TYR:CE2	1:A:300:LEU:HG	2.27	0.69
1:A:205:GLN:H	1:A:205:GLN:NE2	1.91	0.68
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.29	0.68
1:A:328:GLN:NE2	1:A:395:ASP:HA	2.06	0.68
1:A:564:GLU:HB3	1:A:597:THR:CG2	2.22	0.67
1:A:381:MET:HG2	3:A:2054:HOH:O	1.93	0.67
1:A:288:HIS:HB3	1:A:296:VAL:HG12	1.76	0.67
1:A:291:ASN:HB2	1:A:293:THR:HG22	1.79	0.65
1:A:253:VAL:HG23	1:A:254:GLU:HG3	1.78	0.64
1:A:38:LYS:HG3	1:A:139:LEU:HG	1.77	0.64
1:A:668:ARG:HB3	1:A:668:ARG:NH1	2.13	0.64
1:A:604:ASN:HB3	1:A:648:ASN:OD1	1.97	0.64
1:A:221:TRP:CZ2	1:A:223:PRO:HG3	2.33	0.64
1:A:106:LEU:HB3	1:A:301:ARG:NH2	2.11	0.64
1:A:106:LEU:O	1:A:151:MET:O	2.15	0.64
1:A:52:VAL:HB	1:A:130:GLU:HG2	1.80	0.63
1:A:54:THR:OG1	1:A:57:GLU:HG3	1.98	0.63
1:A:553:PRO:O	1:A:554:GLU:HG3	1.99	0.63
1:A:125:MET:CE	1:A:197:LEU:HD12	2.29	0.63
1:A:370:ILE:N	1:A:370:ILE:HD12	2.12	0.63
1:A:328:GLN:HE21	1:A:395:ASP:CA	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:OD2	1:A:418:ALA:HB3	1.99	0.62
1:A:376:THR:HG22	1:A:436:VAL:HG23	1.81	0.62
1:A:301:ARG:HD2	3:A:1025:HOH:O	1.99	0.61
1:A:297:ARG:HD2	1:A:360:GLN:OE1	2.01	0.61
1:A:550:MET:SD	1:A:599:THR:HG23	2.40	0.61
1:A:534:ILE:HD13	1:A:536:VAL:HG23	1.83	0.61
1:A:138:VAL:HG21	1:A:479:ARG:HB2	1.82	0.60
1:A:534:ILE:HD12	1:A:535:VAL:N	2.18	0.59
1:A:605:THR:H	1:A:648:ASN:HD21	1.51	0.58
1:A:645:ASP:HB2	1:A:646:PRO:HD2	1.84	0.58
1:A:329:CYS:O	1:A:332:LEU:HB2	2.03	0.58
1:A:228:ASN:HD22	1:A:228:ASN:C	2.07	0.58
1:A:508:LYS:HA	1:A:558:PHE:CD2	2.38	0.58
1:A:581:SER:O	1:A:620:TYR:HA	2.03	0.58
1:A:178:PHE:HB2	1:A:180:PHE:HE1	1.70	0.57
1:A:74:PRO:HB2	1:A:571:GLU:HB3	1.87	0.57
1:A:622:PHE:CE2	1:A:627:LEU:HD12	2.39	0.56
1:A:81:ARG:HG3	1:A:84:SER:HB3	1.87	0.56
1:A:328:GLN:HG3	1:A:395:ASP:OD1	2.05	0.56
1:A:108:GLY:H	1:A:150:ASN:HD21	1.54	0.56
1:A:537:THR:O	1:A:572:ILE:HA	2.06	0.56
1:A:81:ARG:HG3	1:A:81:ARG:O	2.06	0.56
1:A:644:GLY:HA3	1:A:650:PHE:CZ	2.41	0.55
1:A:426:LEU:CD1	1:A:463:ARG:HH21	2.19	0.55
1:A:343:ARG:O	1:A:397:VAL:HG13	2.07	0.55
1:A:564:GLU:HG2	1:A:596:THR:OG1	2.06	0.55
1:A:257:PRO:HG2	1:A:403:TYR:OH	2.08	0.54
1:A:637:ARG:NH1	1:A:659:ASP:OD2	2.41	0.54
1:A:253:VAL:HG23	1:A:254:GLU:N	2.22	0.53
1:A:148:LEU:C	1:A:148:LEU:HD12	2.27	0.53
1:A:534:ILE:HA	1:A:576:ARG:HB3	1.90	0.53
1:A:305:ASN:ND2	3:A:2013:HOH:O	2.30	0.53
1:A:426:LEU:HD13	1:A:463:ARG:HH21	1.73	0.53
1:A:666:LEU:HG	1:A:675:ASN:HA	1.92	0.52
1:A:666:LEU:HD11	1:A:676:VAL:HG23	1.91	0.52
1:A:106:LEU:CB	1:A:301:ARG:NH2	2.73	0.52
1:A:31:ARG:O	1:A:43:ILE:HG12	2.10	0.52
1:A:185:ASP:CG	1:A:189:VAL:H	2.14	0.51
1:A:44:GLN:HG3	1:A:528:VAL:HG21	1.92	0.51
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.47	0.50
1:A:197:LEU:HD22	1:A:197:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HG3	1:A:261:ARG:CZ	2.41	0.50
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.93	0.50
1:A:28:ILE:O	1:A:31:ARG:HB2	2.12	0.50
1:A:110:LYS:HD3	1:A:112:GLN:OE1	2.11	0.49
1:A:178:PHE:HB2	1:A:180:PHE:CE1	2.47	0.49
1:A:471:ARG:NH2	1:A:514:ALA:HA	2.27	0.49
1:A:413:ASN:O	1:A:415:LYS:HD2	2.12	0.49
1:A:66:VAL:HG11	1:A:149:LEU:HD21	1.93	0.49
1:A:142:LYS:HG2	1:A:431:GLN:OE1	2.12	0.49
1:A:318:CYS:HB3	1:A:337:LYS:HG3	1.93	0.49
1:A:228:ASN:ND2	1:A:228:ASN:C	2.66	0.49
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.27	0.49
1:A:354:ASN:HD22	1:A:355:PHE:N	2.11	0.49
1:A:516:SER:HA	1:A:547:ASN:HB3	1.94	0.49
1:A:125:MET:HE2	1:A:197:LEU:HD12	1.93	0.48
1:A:509:ASP:CG	1:A:511:ASN:HD22	2.16	0.48
1:A:285:SER:HA	1:A:299:ASN:HD22	1.78	0.48
1:A:38:LYS:HD3	3:A:2056:HOH:O	2.13	0.48
1:A:125:MET:HE3	1:A:197:LEU:HD12	1.93	0.48
1:A:354:ASN:HD22	1:A:355:PHE:H	1.61	0.48
1:A:50:ILE:HD12	1:A:131:ILE:O	2.13	0.48
1:A:552:ASP:C	1:A:554:GLU:H	2.17	0.48
1:A:534:ILE:HD12	1:A:534:ILE:C	2.34	0.48
1:A:576:ARG:HD3	1:A:578:LEU:HD21	1.96	0.47
1:A:74:PRO:HG2	1:A:133:ARG:NH1	2.29	0.47
1:A:578:LEU:O	1:A:579:SER:HB3	2.14	0.47
1:A:204:GLN:OE1	1:A:703:GLU:HG3	2.15	0.47
1:A:148:LEU:O	1:A:148:LEU:HD12	2.14	0.47
1:A:560:VAL:HG22	1:A:561:GLU:N	2.29	0.47
1:A:534:ILE:CB	1:A:576:ARG:HB3	2.45	0.47
1:A:111:LEU:HD23	1:A:301:ARG:NH1	2.30	0.47
1:A:537:THR:HG23	3:A:2003:HOH:O	2.15	0.46
1:A:92:ILE:HG22	1:A:93:ARG:HG2	1.97	0.46
1:A:424:ARG:O	1:A:425:ILE:HD13	2.16	0.46
1:A:470:LYS:HB2	1:A:470:LYS:NZ	2.30	0.46
1:A:255:PRO:HG3	1:A:261:ARG:NH2	2.31	0.46
1:A:507:GLY:HA2	1:A:513:PHE:CZ	2.50	0.46
1:A:264:THR:HG22	1:A:703:GLU:OE2	2.15	0.46
1:A:313:TYR:CZ	2:A:718:OES:HC71	2.50	0.46
1:A:42:PRO:HB3	1:A:44:GLN:HE22	1.80	0.46
1:A:465:ALA:HB3	1:A:467:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD12	1:A:150:ASN:H	1.81	0.46
1:A:284:TYR:OH	1:A:298:GLN:NE2	2.48	0.46
1:A:594:GLU:HG2	1:A:595:TYR:N	2.31	0.46
1:A:253:VAL:CG2	1:A:254:GLU:N	2.78	0.46
1:A:45:LYS:HB3	1:A:446:LEU:CD2	2.45	0.46
1:A:249:LYS:HA	1:A:252:THR:OG1	2.17	0.45
1:A:390:TRP:CZ3	1:A:422:PRO:HB3	2.51	0.45
1:A:115:PHE:HD2	1:A:350:GLU:OE2	1.99	0.45
1:A:682:ASN:HB3	1:A:704:ARG:HA	1.97	0.45
1:A:27:THR:HG21	1:A:576:ARG:HA	1.98	0.45
1:A:361:LEU:HD12	3:A:2066:HOH:O	2.15	0.45
1:A:529:PRO:HG2	1:A:532:ARG:O	2.17	0.45
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.52	0.45
1:A:170:THR:OG1	1:A:706:VAL:HG22	2.17	0.45
1:A:688:TYR:HB2	3:A:2037:HOH:O	2.17	0.44
1:A:29:ALA:C	1:A:31:ARG:H	2.19	0.44
1:A:661:LEU:HD12	1:A:662:VAL:N	2.32	0.44
1:A:693:PHE:CE1	1:A:697:GLY:HA3	2.52	0.44
1:A:361:LEU:HD13	1:A:361:LEU:C	2.38	0.44
1:A:552:ASP:O	1:A:554:GLU:N	2.39	0.44
1:A:204:GLN:CD	1:A:703:GLU:HG3	2.38	0.43
1:A:370:ILE:CD1	1:A:370:ILE:N	2.81	0.43
1:A:264:THR:CG2	1:A:703:GLU:OE2	2.66	0.43
1:A:664:TYR:CZ	1:A:668:ARG:HG3	2.51	0.43
1:A:270:ALA:H	1:A:312:VAL:HB	1.84	0.43
1:A:400:LEU:HD11	1:A:405:PRO:HB3	2.01	0.43
1:A:416:ASP:HA	1:A:417:PRO:HD3	1.81	0.43
1:A:680:VAL:HG13	1:A:706:VAL:HG12	1.99	0.43
1:A:534:ILE:CD1	1:A:536:VAL:HG23	2.49	0.43
1:A:589:THR:HB	1:A:613:MET:HB3	2.00	0.43
1:A:479:ARG:HG3	1:A:497:SER:HB3	2.00	0.43
1:A:630:LEU:HD13	1:A:631:THR:N	2.33	0.43
1:A:66:VAL:HG23	3:A:1002:HOH:O	2.17	0.43
1:A:205:GLN:HE21	1:A:205:GLN:H	1.65	0.43
1:A:471:ARG:HH21	1:A:515:PRO:HD3	1.82	0.43
1:A:575:LYS:C	1:A:576:ARG:HG3	2.39	0.43
1:A:663:ARG:NH2	3:A:2048:HOH:O	2.51	0.43
1:A:116:TYR:OH	2:A:718:OES:HC82	2.19	0.42
1:A:149:LEU:HD12	1:A:150:ASN:N	2.34	0.42
1:A:690:ALA:O	1:A:691:SER:HB3	2.19	0.42
1:A:425:ILE:HG22	1:A:426:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:O	1:A:38:LYS:HB2	2.19	0.42
1:A:383:MET:HE3	1:A:385:ASN:N	2.35	0.42
1:A:273:ASN:HA	1:A:273:ASN:HD22	1.61	0.42
1:A:446:LEU:HB3	1:A:483:ASN:HB2	2.01	0.42
1:A:297:ARG:HH22	1:A:362:GLN:NE2	2.17	0.42
1:A:138:VAL:HG21	1:A:479:ARG:CB	2.47	0.42
1:A:572:ILE:HD12	1:A:573:GLU:N	2.35	0.42
1:A:300:LEU:HD12	1:A:300:LEU:C	2.40	0.41
1:A:383:MET:HE3	1:A:384:ARG:C	2.41	0.41
1:A:471:ARG:NH2	1:A:515:PRO:HD3	2.34	0.41
1:A:185:ASP:CG	1:A:188:GLY:H	2.24	0.41
1:A:116:TYR:OH	2:A:718:OES:C8	2.69	0.41
1:A:333:ALA:O	1:A:335:ALA:N	2.50	0.41
1:A:159:GLU:N	1:A:159:GLU:OE1	2.53	0.41
1:A:44:GLN:HG2	1:A:528:VAL:HB	2.03	0.41
1:A:158:THR:HG22	1:A:159:GLU:CD	2.40	0.41
1:A:44:GLN:H	1:A:44:GLN:NE2	2.19	0.41
1:A:176:THR:CG2	2:A:715:OES:HC12	2.50	0.40
1:A:710:ALA:HB2	2:A:716:OES:HC72	2.03	0.40
1:A:407:ASN:HB3	3:A:2034:HOH:O	2.20	0.40
1:A:500:PHE:CE2	1:A:502:PRO:HD3	2.56	0.40
1:A:668:ARG:HB3	1:A:668:ARG:CZ	2.51	0.40
1:A:556:SER:C	1:A:558:PHE:H	2.24	0.40
1:A:258:ASN:HB3	1:A:403:TYR:OH	2.20	0.40
1:A:81:ARG:O	1:A:81:ARG:CG	2.70	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	693/714 (97%)	643 (93%)	45 (6%)	5 (1%)	22 40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	GLY
1	A	170	THR
1	A	599	THR
1	A	21	ALA
1	A	136	VAL

### 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	578/593 (98%)	533 (92%)	45 (8%)	12 22

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	52	VAL
1	A	80	THR
1	A	93	ARG
1	A	106	LEU
1	A	117	ASN
1	A	118	ASP
1	A	120	VAL
1	A	139	LEU
1	A	186	ASP
1	A	195	THR
1	A	197	LEU
1	A	205	GLN
1	A	228	ASN
1	A	247	LEU
1	A	264	THR
1	A	275	TYR
1	A	291	ASN
1	A	293	THR
1	A	300	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	305	ASN
1	A	327	LYS
1	A	354	ASN
1	A	381	MET
1	A	383	MET
1	A	384	ARG
1	A	397	VAL
1	A	449	LEU
1	A	461	LEU
1	A	467	THR
1	A	470	LYS
1	A	543	LEU
1	A	544	THR
1	A	572	ILE
1	A	576	ARG
1	A	585	VAL
1	A	591	THR
1	A	597	THR
1	A	613	MET
1	A	634	THR
1	A	668	ARG
1	A	686	ARG
1	A	689	VAL
1	A	694	ASN
1	A	711	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	32	GLN
1	A	44	GLN
1	A	61	HIS
1	A	89	HIS
1	A	114	ASN
1	A	117	ASN
1	A	150	ASN
1	A	175	GLN
1	A	205	GLN
1	A	228	ASN
1	A	236	GLN
1	A	273	ASN
1	A	298	GLN

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	305	ASN
1	A	310	ASN
1	A	323	ASN
1	A	328	GLN
1	A	354	ASN
1	A	362	GLN
1	A	385	ASN
1	A	388	ASN
1	A	407	ASN
1	A	441	GLN
1	A	511	ASN
1	A	547	ASN
1	A	604	ASN
1	A	694	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

7 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	OES	A	721	-	11,12,12	0.41	0	11,12,12	1.89	2 (18%)
2	OES	A	715	-	11,12,12	0.42	0	11,12,12	1.75	2 (18%)
2	OES	A	720	-	11,12,12	0.42	0	11,12,12	1.71	2 (18%)
2	OES	A	716	-	11,12,12	0.52	0	11,12,12	1.84	2 (18%)
2	OES	A	718	-	11,12,12	0.49	0	11,12,12	2.09	2 (18%)
2	OES	A	717	-	11,12,12	0.41	0	11,12,12	1.68	2 (18%)
2	OES	A	719	-	11,12,12	0.43	0	11,12,12	1.73	2 (18%)

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	OES	A	721	-	-	7/11/11/11	-
2	OES	A	715	-	-	6/11/11/11	-
2	OES	A	720	-	-	7/11/11/11	-
2	OES	A	716	-	-	5/11/11/11	-
2	OES	A	718	-	-	6/11/11/11	-
2	OES	A	717	-	-	6/11/11/11	-
2	OES	A	719	-	-	7/11/11/11	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	718	OES	C22-S2-C8	5.97	110.13	97.24
2	A	721	OES	C22-S2-C8	5.39	108.87	97.24
2	A	716	OES	C22-S2-C8	5.21	108.49	97.24
2	A	715	OES	C22-S2-C8	4.90	107.83	97.24
2	A	719	OES	C22-S2-C8	4.74	107.47	97.24
2	A	717	OES	C22-S2-C8	4.61	107.19	97.24
2	A	720	OES	C22-S2-C8	4.58	107.14	97.24
2	A	718	OES	O2-S2-C8	-3.06	98.82	105.84
2	A	720	OES	O2-S2-C8	-2.73	99.57	105.84
2	A	721	OES	O2-S2-C8	-2.62	99.82	105.84
2	A	716	OES	O2-S2-C8	-2.54	100.00	105.84
2	A	719	OES	O2-S2-C8	-2.50	100.11	105.84
2	A	715	OES	O2-S2-C8	-2.44	100.23	105.84

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	717	OES	O2-S2-C8	-2.43	100.26	105.84

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	719	OES	C3-C4-C5-C6
2	A	721	OES	C3-C4-C5-C6
2	A	718	OES	C3-C4-C5-C6
2	A	717	OES	C6-C7-C8-S2
2	A	717	OES	C3-C4-C5-C6
2	A	721	OES	C23-C22-S2-O2
2	A	715	OES	C23-C22-S2-O2
2	A	720	OES	C23-C22-S2-O2
2	A	716	OES	C23-C22-S2-O2
2	A	718	OES	C23-C22-S2-O2
2	A	717	OES	C23-C22-S2-O2
2	A	719	OES	C23-C22-S2-O2
2	A	718	OES	C1-C2-C3-C4
2	A	715	OES	C2-C3-C4-C5
2	A	716	OES	C1-C2-C3-C4
2	A	720	OES	C1-C2-C3-C4
2	A	721	OES	C23-C22-S2-C8
2	A	715	OES	C23-C22-S2-C8
2	A	720	OES	C23-C22-S2-C8
2	A	716	OES	C23-C22-S2-C8
2	A	718	OES	C23-C22-S2-C8
2	A	717	OES	C23-C22-S2-C8
2	A	719	OES	C23-C22-S2-C8
2	A	721	OES	C6-C7-C8-S2
2	A	721	OES	C7-C8-S2-O2
2	A	715	OES	C7-C8-S2-O2
2	A	720	OES	C7-C8-S2-O2
2	A	716	OES	C7-C8-S2-O2
2	A	718	OES	C7-C8-S2-O2
2	A	717	OES	C7-C8-S2-O2
2	A	719	OES	C7-C8-S2-O2
2	A	721	OES	C7-C8-S2-C22
2	A	715	OES	C7-C8-S2-C22
2	A	720	OES	C7-C8-S2-C22
2	A	716	OES	C7-C8-S2-C22
2	A	718	OES	C7-C8-S2-C22

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Mol	Chain	Res	Type	Atoms
2	A	717	OES	C7-C8-S2-C22
2	A	719	OES	C7-C8-S2-C22
2	A	720	OES	C3-C4-C5-C6
2	A	719	OES	C2-C3-C4-C5
2	A	715	OES	C3-C4-C5-C6
2	A	720	OES	C2-C3-C4-C5
2	A	721	OES	C2-C3-C4-C5
2	A	719	OES	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	715	OES	1	0
2	A	716	OES	1	0
2	A	718	OES	3	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, 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	695/714 (97%)	0.08	33 (4%) 31 34	29, 51, 79, 110	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	GLY	6.4
1	A	557	PHE	5.0
1	A	623	PHE	4.8
1	A	558	PHE	4.6
1	A	556	SER	4.2
1	A	507	GLY	4.2
1	A	186	ASP	3.5
1	A	418	ALA	3.1
1	A	366	ALA	3.0
1	A	508	LYS	3.0
1	A	158	THR	2.9
1	A	532	ARG	2.9
1	A	292	ASP	2.9
1	A	629	GLY	2.7
1	A	603	GLY	2.6
1	A	559	SER	2.5
1	A	624	ASP	2.5
1	A	580	ALA	2.5
1	A	325	TYR	2.5
1	A	185	ASP	2.5
1	A	531	ASP	2.5
1	A	370	ILE	2.4
1	A	190	TYR	2.4
1	A	488	ASN	2.4
1	A	513	PHE	2.4
1	A	419	ASN	2.3
1	A	628	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	560	VAL	2.2
1	A	184	LEU	2.2
1	A	643	TYR	2.1
1	A	576	ARG	2.1
1	A	157	THR	2.1
1	A	487	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. 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(Å <sup>2</sup> )	Q<0.9
2	OES	A	720	13/13	0.70	0.39	76,90,116,117	0
2	OES	A	717	13/13	0.80	0.27	78,82,107,109	0
2	OES	A	716	13/13	0.82	0.41	40,71,99,103	0
2	OES	A	721	13/13	0.82	0.28	65,86,111,112	0
2	OES	A	715	13/13	0.85	0.26	53,69,97,99	0
2	OES	A	719	13/13	0.88	0.17	67,81,110,114	0
2	OES	A	718	13/13	0.93	0.43	67,72,95,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.