



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:27 PM EDT

PDB ID : 1BY5 / pdb_00001by5
Title : FHUA FROM E. COLI, WITH ITS LIGAND FERRICHROME
Authors : Locher, K.P.; Rees, B.; Koebnik, R.; Mitschler, A.; Moulinier, L.; Rosenbusch, J.P.; Moras, D.
Deposited on : 1998-10-23
Resolution : 2.60 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

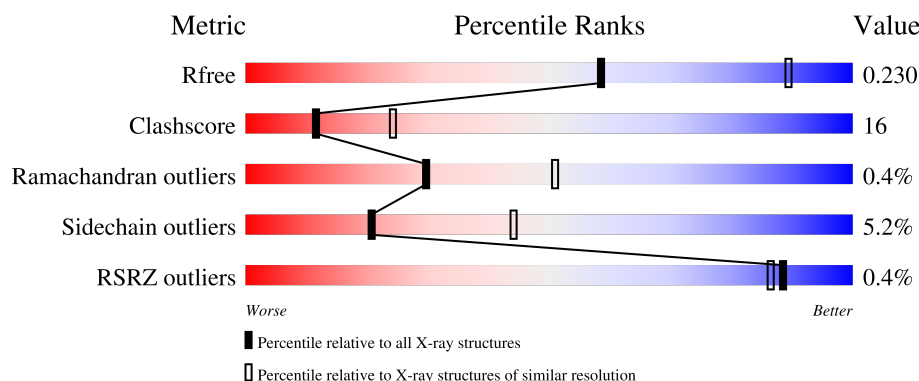
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	714	 69% 25% . .
2	B	6	 50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5749 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 FERRIC HYDROXAMATE UPTAKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5453	3435	926	1078	14	0	0	0

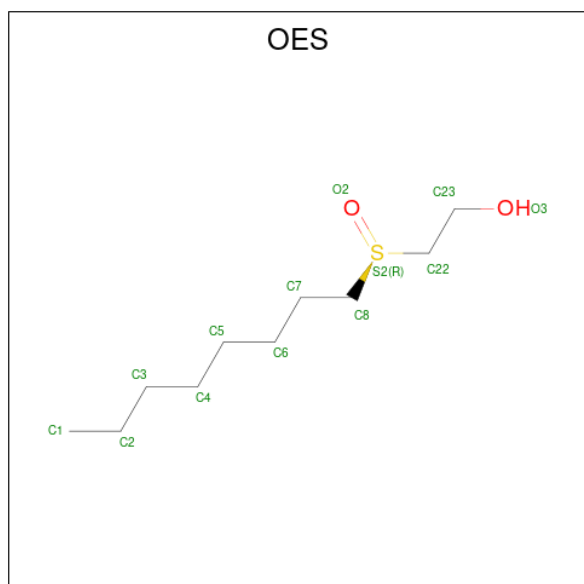
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called FERRICHROME.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	48	27	9	12	0	0	0

- Molecule 3 is N-OCTYL-2-HYDROXYETHYL SULFOXIDE (CCD ID: OES) (formula: $C_{10}H_{22}O_2S$).



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

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		

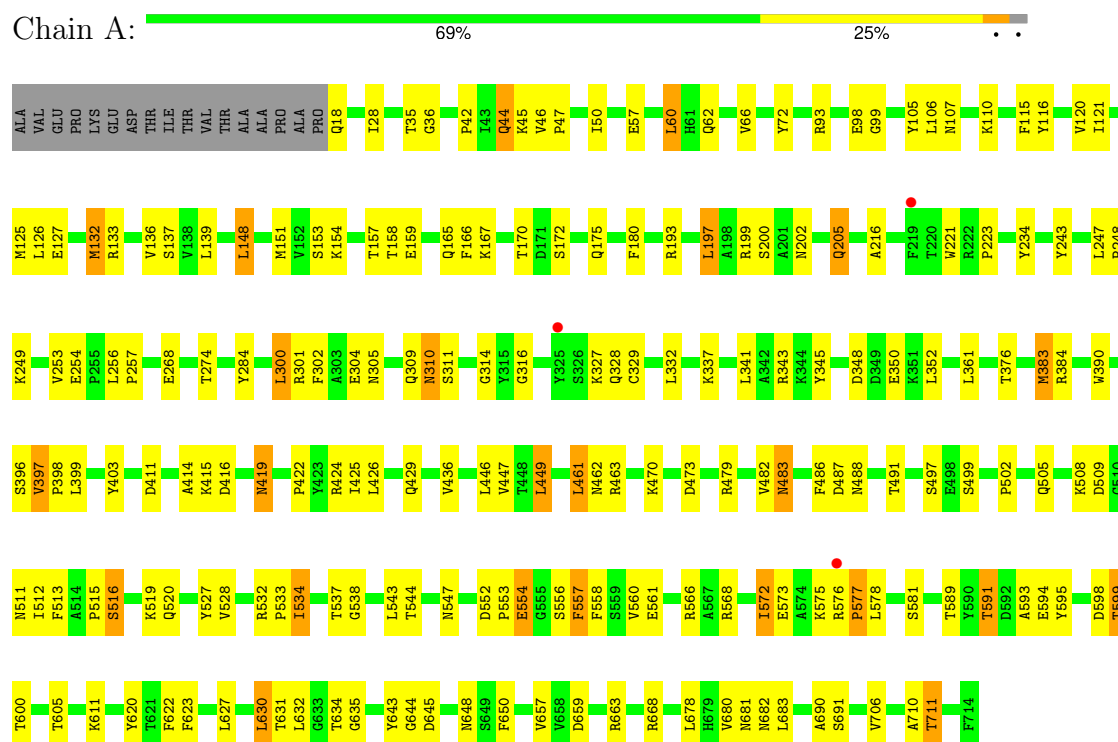
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		

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: FERRIC HYDROXAMATE UPTAKE PROTEIN



• Molecule 2: FERRICHROME



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.20Å 89.40Å 89.90Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 12.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.5 (12.00-2.60) 88.5 (12.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.57Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.184 , 0.229 0.187 , 0.230	Depositor DCC
R_{free} test set	1561 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5749	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 5.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AHO, FE, 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	0.43	0/5588	0.86	5/7593 (0.1%)
2	B	1.48	0/9	1.02	0/6
All	All	0.43	0/5597	0.86	5/7599 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	SER	N-CA-C	6.78	119.45	108.34
1	A	516	SER	N-CA-C	-5.67	103.22	110.53
1	A	310	ASN	N-CA-C	-5.57	96.05	107.70
1	A	127	GLU	N-CA-C	-5.55	104.74	112.45
1	A	554	GLU	N-CA-C	-5.47	106.28	113.12

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	5453	0	5176	175	0
2	B	48	0	27	0	0
3	A	104	0	176	4	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	143	0	0	4	0
All	All	5749	0	5379	176	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 16.

All (176) 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:66:VAL:HG21	1:A:151:MET:HE3	1.24	1.08
1:A:533:PRO:O	1:A:577:PRO:HD2	1.74	0.88
1:A:426:LEU:HB2	1:A:463:ARG:HH12	1.40	0.85
1:A:98:GLU:HB2	5:A:1015:HOH:O	1.81	0.81
1:A:136:VAL:HG21	1:A:148:LEU:HD13	1.71	0.72
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.71	0.71
1:A:121:ILE:HB	1:A:151:MET:HE1	1.74	0.69
1:A:121:ILE:HB	1:A:151:MET:CE	2.23	0.69
1:A:107:ASN:HD21	1:A:153:SER:H	1.41	0.68
1:A:126:LEU:HD11	1:A:151:MET:HE2	1.76	0.67
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.77	0.67
1:A:170:THR:HG23	1:A:706:VAL:CG1	2.25	0.67
1:A:383:MET:HG3	1:A:429:GLN:HB2	1.77	0.66
1:A:125:MET:HE3	1:A:216:ALA:HB2	1.78	0.66
1:A:352:LEU:HG	1:A:383:MET:HE1	1.79	0.65
1:A:581:SER:HB3	1:A:623:PHE:CE2	2.32	0.64
1:A:534:ILE:HB	1:A:576:ARG:HD3	1.79	0.64
1:A:376:THR:HG22	1:A:436:VAL:HG23	1.80	0.63
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.64	0.63
1:A:532:ARG:HB3	1:A:534:ILE:HG23	1.81	0.63
1:A:257:PRO:HG2	1:A:403:TYR:OH	1.99	0.63
1:A:657:VAL:HG13	1:A:682:ASN:HA	1.82	0.62
1:A:57:GLU:O	1:A:60:LEU:HB2	2.01	0.61
1:A:126:LEU:HD11	1:A:151:MET:CE	2.30	0.61
1:A:483:ASN:HD22	1:A:483:ASN:N	1.99	0.60
1:A:300:LEU:C	1:A:300:LEU:HD12	2.26	0.60
1:A:148:LEU:HD23	1:A:148:LEU:C	2.27	0.60
1:A:411:ASP:OD2	1:A:414:ALA:HB2	2.01	0.60
1:A:520:GLN:HB2	1:A:543:LEU:HD13	1.84	0.60
1:A:552:ASP:OD1	1:A:554:GLU:HG2	2.02	0.59
1:A:560:VAL:HG22	1:A:561:GLU:N	2.17	0.59
1:A:578:LEU:H	1:A:578:LEU:CD1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ARG:HG3	1:A:668:ARG:HH11	1.67	0.59
1:A:482:VAL:C	1:A:483:ASN:HD22	2.10	0.59
1:A:165:GLN:HE21	1:A:711:THR:CG2	2.15	0.59
1:A:578:LEU:HD12	1:A:578:LEU:N	2.18	0.58
1:A:256:LEU:HB3	1:A:257:PRO:HD2	1.85	0.58
1:A:593:ALA:O	1:A:605:THR:HG22	2.03	0.58
1:A:352:LEU:HG	1:A:383:MET:CE	2.33	0.58
1:A:463:ARG:HG3	1:A:463:ARG:HH11	1.68	0.58
1:A:314:GLY:HA2	1:A:343:ARG:HG2	1.85	0.58
1:A:170:THR:HG23	1:A:706:VAL:HG12	1.86	0.57
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.39	0.57
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.19	0.57
1:A:35:THR:HG22	1:A:132:MET:HG3	1.85	0.57
1:A:62:GLN:OE1	1:A:167:LYS:HE2	2.04	0.57
1:A:106:LEU:HB3	1:A:301:ARG:NH2	2.20	0.57
1:A:446:LEU:HD23	1:A:447:VAL:N	2.19	0.57
1:A:426:LEU:HB2	1:A:463:ARG:NH1	2.16	0.56
1:A:589:THR:HG22	1:A:591:THR:HG22	1.86	0.56
1:A:170:THR:CG2	1:A:706:VAL:HG12	2.36	0.56
1:A:710:ALA:HB2	3:A:719:OES:HC62	1.87	0.55
3:A:718:OES:O2	3:A:722:OES:HC82	2.07	0.55
1:A:253:VAL:HG23	1:A:254:GLU:HG2	1.89	0.55
1:A:66:VAL:HG21	1:A:151:MET:CE	2.16	0.55
1:A:534:ILE:HB	1:A:576:ARG:CD	2.37	0.55
1:A:502:PRO:HA	1:A:515:PRO:HB3	1.88	0.55
1:A:172:SER:HB2	1:A:202:ASN:ND2	2.21	0.54
1:A:36:GLY:HA2	1:A:132:MET:HE2	1.90	0.54
1:A:47:PRO:HB3	1:A:483:ASN:HD21	1.73	0.54
1:A:383:MET:HE2	1:A:384:ARG:N	2.22	0.54
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.43	0.54
1:A:578:LEU:H	1:A:578:LEU:HD12	1.73	0.54
1:A:644:GLY:HA3	1:A:650:PHE:CZ	2.42	0.54
1:A:560:VAL:HG22	1:A:561:GLU:H	1.72	0.54
1:A:566:ARG:HH11	1:A:566:ARG:HG3	1.74	0.53
1:A:125:MET:HE3	1:A:216:ALA:CB	2.40	0.52
1:A:165:GLN:HE21	1:A:711:THR:HG21	1.74	0.52
1:A:630:LEU:HD13	1:A:631:THR:N	2.25	0.52
1:A:630:LEU:HD12	1:A:632:LEU:HG	1.91	0.52
1:A:249:LYS:HB2	1:A:253:VAL:CG2	2.40	0.52
1:A:175:GLN:OE1	1:A:199:ARG:HD3	2.10	0.52
1:A:416:ASP:HB3	1:A:419:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:SER:HB3	1:A:623:PHE:HE2	1.71	0.52
1:A:197:LEU:C	1:A:197:LEU:HD22	2.34	0.51
1:A:305:ASN:HB3	5:A:3008:HOH:O	2.11	0.51
1:A:509:ASP:OD1	1:A:511:ASN:HB2	2.10	0.51
1:A:329:CYS:O	1:A:337:LYS:HE2	2.11	0.51
1:A:248:PRO:HB3	1:A:316:GLY:HA2	1.93	0.51
1:A:301:ARG:HG2	1:A:302:PHE:N	2.26	0.50
1:A:249:LYS:HB2	1:A:253:VAL:HG22	1.94	0.50
1:A:532:ARG:HH11	1:A:532:ARG:HG3	1.77	0.50
1:A:157:THR:HG22	1:A:158:THR:N	2.26	0.50
1:A:390:TRP:CZ3	1:A:422:PRO:HB3	2.46	0.50
1:A:473:ASP:OD2	1:A:515:PRO:HD3	2.12	0.50
1:A:573:GLU:OE2	1:A:575:LYS:HE3	2.12	0.49
1:A:508:LYS:HE2	1:A:556:SER:OG	2.13	0.49
1:A:419:ASN:HD22	1:A:419:ASN:C	2.21	0.49
1:A:622:PHE:CE2	1:A:627:LEU:HD12	2.48	0.49
1:A:553:PRO:HG3	1:A:599:THR:HG21	1.95	0.49
1:A:253:VAL:HG23	1:A:254:GLU:N	2.27	0.48
1:A:680:VAL:HG11	1:A:683:LEU:HD13	1.96	0.48
1:A:45:LYS:HE2	1:A:446:LEU:CD1	2.44	0.48
1:A:284:TYR:CE2	1:A:300:LEU:HG	2.49	0.48
1:A:348:ASP:OD2	1:A:350:GLU:HG3	2.14	0.47
1:A:180:PHE:O	1:A:193:ARG:HA	2.14	0.47
1:A:578:LEU:CD1	1:A:578:LEU:N	2.75	0.47
1:A:631:THR:HB	1:A:663:ARG:HB3	1.97	0.47
1:A:148:LEU:HD23	1:A:148:LEU:O	2.15	0.47
1:A:486:PHE:C	1:A:488:ASN:H	2.22	0.47
1:A:345:TYR:HE1	1:A:396:SER:HB2	1.79	0.47
1:A:505:GLN:HB2	1:A:513:PHE:HD2	1.80	0.47
1:A:45:LYS:HE2	1:A:446:LEU:HD12	1.96	0.47
1:A:479:ARG:HG3	1:A:497:SER:HB3	1.96	0.47
1:A:527:TYR:CE2	1:A:534:ILE:HD11	2.49	0.46
1:A:44:GLN:HG2	1:A:528:VAL:HB	1.96	0.46
1:A:537:THR:O	1:A:572:ILE:HA	2.16	0.46
1:A:425:ILE:HD13	1:A:462:ASN:HA	1.98	0.46
1:A:581:SER:O	1:A:620:TYR:HA	2.16	0.46
1:A:576:ARG:HG3	1:A:578:LEU:CD1	2.46	0.46
1:A:446:LEU:HD23	1:A:446:LEU:C	2.41	0.46
1:A:137:SER:HB2	1:A:499:SER:HA	1.98	0.46
1:A:505:GLN:HB2	1:A:513:PHE:CD2	2.51	0.45
1:A:534:ILE:HB	1:A:576:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:CG	1:A:383:MET:HE1	2.46	0.45
1:A:345:TYR:CE1	1:A:396:SER:HB2	2.51	0.45
1:A:627:LEU:O	1:A:630:LEU:HB2	2.16	0.45
1:A:126:LEU:HD22	1:A:151:MET:HB3	1.99	0.45
1:A:105:TYR:CE1	1:A:148:LEU:HD12	2.52	0.45
1:A:50:ILE:HG12	1:A:132:MET:HG2	1.99	0.44
1:A:200:SER:HB2	3:A:715:OES:HC82	1.98	0.44
1:A:645:ASP:OD1	1:A:648:ASN:N	2.50	0.44
1:A:121:ILE:HB	1:A:151:MET:HE2	1.99	0.44
1:A:516:SER:HA	1:A:547:ASN:HB3	2.00	0.44
1:A:532:ARG:HG3	1:A:532:ARG:NH1	2.32	0.44
1:A:45:LYS:CE	1:A:446:LEU:HD12	2.48	0.44
1:A:390:TRP:CE2	1:A:415:LYS:HB3	2.53	0.44
1:A:309:GLN:HG2	1:A:348:ASP:HB3	2.00	0.44
1:A:328:GLN:HE22	1:A:398:PRO:HA	1.83	0.44
1:A:706:VAL:HG13	1:A:706:VAL:O	2.18	0.44
1:A:534:ILE:HB	1:A:576:ARG:CB	2.48	0.44
1:A:537:THR:HG22	1:A:538:GLY:N	2.33	0.44
1:A:343:ARG:HB2	1:A:397:VAL:CG2	2.48	0.43
1:A:42:PRO:HB3	1:A:44:GLN:HE22	1.83	0.43
1:A:668:ARG:HG3	1:A:668:ARG:NH1	2.33	0.43
1:A:690:ALA:O	1:A:691:SER:HB3	2.18	0.43
1:A:659:ASP:OD1	1:A:681:ASN:HA	2.18	0.43
1:A:505:GLN:O	1:A:512:ILE:HA	2.18	0.43
1:A:533:PRO:HB2	1:A:577:PRO:CG	2.49	0.43
1:A:566:ARG:HD3	1:A:568:ARG:HE	1.82	0.43
1:A:390:TRP:CZ2	1:A:415:LYS:HB3	2.54	0.42
1:A:598:ASP:C	1:A:600:THR:H	2.26	0.42
1:A:663:ARG:NE	5:A:6039:HOH:O	2.40	0.42
1:A:419:ASN:C	1:A:419:ASN:ND2	2.78	0.42
1:A:470:LYS:HB3	1:A:470:LYS:NZ	2.34	0.42
1:A:332:LEU:HD11	1:A:399:LEU:HD13	2.00	0.42
1:A:424:ARG:O	1:A:425:ILE:HD13	2.18	0.42
1:A:634:THR:HG22	1:A:635:GLY:N	2.35	0.42
1:A:36:GLY:HA3	1:A:50:ILE:HD11	2.01	0.42
1:A:46:VAL:HG11	1:A:50:ILE:HD12	2.01	0.42
1:A:98:GLU:HG2	1:A:99:GLY:N	2.35	0.42
1:A:166:PHE:HB3	3:A:719:OES:H221	2.01	0.42
1:A:532:ARG:HA	1:A:533:PRO:HD3	1.85	0.42
1:A:159:GLU:OE1	1:A:159:GLU:N	2.47	0.41
1:A:577:PRO:HG2	1:A:577:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:HE1	5:A:6015:HOH:O	2.02	0.41
1:A:557:PHE:HD1	1:A:557:PHE:HA	1.75	0.41
1:A:115:PHE:HB3	1:A:116:TYR:H	1.70	0.41
1:A:594:GLU:HG2	1:A:595:TYR:N	2.36	0.41
1:A:560:VAL:CG2	1:A:561:GLU:N	2.84	0.41
1:A:18:GLN:NE2	1:A:18:GLN:HA	2.36	0.41
1:A:106:LEU:O	1:A:301:ARG:NH2	2.53	0.41
1:A:461:LEU:C	1:A:461:LEU:HD13	2.45	0.41
1:A:556:SER:C	1:A:558:PHE:H	2.29	0.41
1:A:605:THR:OG1	1:A:643:TYR:CD2	2.74	0.41
1:A:680:VAL:HG11	1:A:683:LEU:CD1	2.51	0.41
1:A:221:TRP:CE2	1:A:223:PRO:HD3	2.56	0.41
1:A:300:LEU:C	1:A:300:LEU:CD1	2.92	0.41
1:A:304:GLU:HA	1:A:352:LEU:O	2.21	0.41
1:A:426:LEU:CB	1:A:463:ARG:HH12	2.21	0.41
1:A:327:LYS:HB3	1:A:327:LYS:NZ	2.36	0.40
1:A:534:ILE:HA	1:A:576:ARG:HB3	2.02	0.40
1:A:352:LEU:CD1	1:A:383:MET:HE1	2.51	0.40
1:A:449:LEU:HD22	1:A:449:LEU:HA	1.94	0.40
1:A:93:ARG:CZ	1:A:133:ARG:HB3	2.52	0.40
1:A:611:LYS:HE3	1:A:611:LYS:HB2	1.98	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	695/714 (97%)	653 (94%)	39 (6%)	3 (0%)	30	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	ASP
1	A	577	PRO
1	A	599	THR

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	580/593 (98%)	550 (95%)	30 (5%)	21	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	44	GLN
1	A	60	LEU
1	A	120	VAL
1	A	132	MET
1	A	139	LEU
1	A	148	LEU
1	A	197	LEU
1	A	205	GLN
1	A	247	LEU
1	A	268	GLU
1	A	300	LEU
1	A	341	LEU
1	A	361	LEU
1	A	383	MET
1	A	397	VAL
1	A	419	ASN
1	A	449	LEU
1	A	461	LEU
1	A	483	ASN
1	A	491	THR
1	A	519	LYS
1	A	534	ILE
1	A	544	THR

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Mol	Chain	Res	Type
1	A	557	PHE
1	A	572	ILE
1	A	591	THR
1	A	630	LEU
1	A	678	LEU
1	A	711	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	44	GLN
1	A	85	ASN
1	A	100	GLN
1	A	107	ASN
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	310	ASN
1	A	323	ASN
1	A	328	GLN
1	A	339	HIS
1	A	354	ASN
1	A	419	ASN
1	A	458	GLN
1	A	483	ASN
1	A	511	ASN
1	A	604	ASN
1	A	679	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	AHO	B	803	4,2	9,11,12	1.28	1 (11%)	4,13,15	0.84	0
2	AHO	B	801	4,2	9,11,12	0.89	1 (11%)	4,13,15	0.86	0
2	AHO	B	802	4,2	9,11,12	1.87	1 (11%)	4,13,15	1.26	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	AHO	B	803	4,2	-	2/11/12/14	-
2	AHO	B	801	4,2	-	6/11/12/14	-
2	AHO	B	802	4,2	-	3/11/12/14	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	AHO	O2-N2	-4.80	1.36	1.40
2	B	803	AHO	C3-CA	3.23	1.58	1.53
2	B	801	AHO	O2-N2	2.09	1.41	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	AHO	O-C-CA-C3
2	B	801	AHO	C4-C5-N2-O2
2	B	802	AHO	O-C-CA-C3
2	B	801	AHO	C4-C5-N2-C6
2	B	801	AHO	C4-C3-CA-C
2	B	801	AHO	C7-C6-N2-O2
2	B	802	AHO	C7-C6-N2-O2
2	B	803	AHO	C7-C6-N2-O2

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Mol	Chain	Res	Type	Atoms
2	B	801	AHO	O3-C6-N2-O2
2	B	802	AHO	O3-C6-N2-O2
2	B	803	AHO	O3-C6-N2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
3	OES	A	722	-	12,12,12	1.26	1 (8%)	11,12,12	1.91	2 (18%)
3	OES	A	720	-	12,12,12	1.13	1 (8%)	11,12,12	1.97	2 (18%)
3	OES	A	715	-	12,12,12	1.31	1 (8%)	11,12,12	1.93	3 (27%)
3	OES	A	721	-	12,12,12	1.12	1 (8%)	11,12,12	1.73	2 (18%)
3	OES	A	716	-	12,12,12	1.21	1 (8%)	11,12,12	1.76	2 (18%)
3	OES	A	717	-	12,12,12	1.15	1 (8%)	11,12,12	2.12	2 (18%)
3	OES	A	718	-	12,12,12	1.20	1 (8%)	11,12,12	1.99	2 (18%)
3	OES	A	719	-	12,12,12	1.11	1 (8%)	11,12,12	1.93	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
3	OES	A	722	-	-	6/11/11/11	-
3	OES	A	720	-	-	7/11/11/11	-
3	OES	A	715	-	-	8/11/11/11	-
3	OES	A	721	-	-	6/11/11/11	-
3	OES	A	716	-	-	6/11/11/11	-
3	OES	A	717	-	-	7/11/11/11	-
3	OES	A	718	-	-	6/11/11/11	-
3	OES	A	719	-	-	8/11/11/11	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	715	OES	C22-C23	-4.23	1.46	1.51
3	A	722	OES	C22-C23	-4.05	1.46	1.51
3	A	716	OES	C22-C23	-4.04	1.46	1.51
3	A	718	OES	C22-C23	-3.91	1.46	1.51
3	A	717	OES	C22-C23	-3.69	1.46	1.51
3	A	720	OES	C22-C23	-3.66	1.46	1.51
3	A	719	OES	C22-C23	-3.62	1.46	1.51
3	A	721	OES	C22-C23	-3.60	1.46	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	717	OES	C22-S2-C8	5.95	109.69	97.40
3	A	720	OES	C22-S2-C8	5.52	108.81	97.40
3	A	718	OES	C22-S2-C8	5.46	108.68	97.40
3	A	722	OES	C22-S2-C8	5.36	108.48	97.40
3	A	719	OES	C22-S2-C8	5.29	108.34	97.40
3	A	715	OES	C22-S2-C8	5.15	108.04	97.40
3	A	716	OES	C22-S2-C8	4.85	107.43	97.40
3	A	721	OES	C22-S2-C8	4.72	107.15	97.40
3	A	717	OES	O2-S2-C8	-3.12	98.82	105.73
3	A	718	OES	O2-S2-C8	-3.10	98.85	105.73
3	A	719	OES	O2-S2-C8	-2.98	99.12	105.73
3	A	720	OES	O2-S2-C8	-2.86	99.39	105.73
3	A	716	OES	O2-S2-C8	-2.52	100.15	105.73
3	A	721	OES	O2-S2-C8	-2.50	100.19	105.73
3	A	722	OES	O2-S2-C8	-2.50	100.20	105.73
3	A	715	OES	O2-S2-C8	-2.34	100.55	105.73
3	A	715	OES	C8-C7-C6	2.03	118.11	112.17

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	715	OES	C6-C7-C8-S2
3	A	715	OES	C23-C22-S2-O2
3	A	716	OES	C23-C22-S2-O2
3	A	717	OES	C6-C7-C8-S2
3	A	717	OES	C23-C22-S2-O2
3	A	718	OES	C23-C22-S2-O2
3	A	719	OES	C6-C7-C8-S2
3	A	719	OES	C23-C22-S2-O2
3	A	720	OES	C23-C22-S2-O2
3	A	721	OES	C6-C7-C8-S2
3	A	721	OES	C23-C22-S2-O2
3	A	722	OES	C23-C22-S2-O2
3	A	722	OES	C2-C3-C4-C5
3	A	719	OES	C2-C3-C4-C5
3	A	718	OES	C3-C4-C5-C6
3	A	717	OES	C3-C4-C5-C6
3	A	715	OES	C3-C4-C5-C6
3	A	720	OES	C2-C3-C4-C5
3	A	715	OES	C2-C3-C4-C5
3	A	716	OES	C2-C3-C4-C5
3	A	721	OES	C3-C4-C5-C6
3	A	719	OES	C1-C2-C3-C4
3	A	720	OES	C3-C4-C5-C6
3	A	716	OES	C23-C22-S2-C8
3	A	717	OES	C23-C22-S2-C8
3	A	718	OES	C23-C22-S2-C8
3	A	719	OES	C23-C22-S2-C8
3	A	720	OES	C23-C22-S2-C8
3	A	721	OES	C23-C22-S2-C8
3	A	715	OES	C7-C8-S2-O2
3	A	716	OES	C7-C8-S2-O2
3	A	717	OES	C7-C8-S2-O2
3	A	718	OES	C7-C8-S2-O2
3	A	719	OES	C7-C8-S2-O2
3	A	720	OES	C7-C8-S2-O2
3	A	721	OES	C7-C8-S2-O2
3	A	722	OES	C7-C8-S2-O2
3	A	715	OES	C7-C8-S2-C22
3	A	716	OES	C7-C8-S2-C22
3	A	717	OES	C7-C8-S2-C22

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Mol	Chain	Res	Type	Atoms
3	A	718	OES	C7-C8-S2-C22
3	A	719	OES	C7-C8-S2-C22
3	A	720	OES	C7-C8-S2-C22
3	A	721	OES	C7-C8-S2-C22
3	A	722	OES	C7-C8-S2-C22
3	A	715	OES	C1-C2-C3-C4
3	A	722	OES	C3-C4-C5-C6
3	A	715	OES	C23-C22-S2-C8
3	A	722	OES	C23-C22-S2-C8
3	A	718	OES	C2-C3-C4-C5
3	A	717	OES	C1-C2-C3-C4
3	A	716	OES	C3-C4-C5-C6
3	A	720	OES	C1-C2-C3-C4
3	A	719	OES	C3-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	722	OES	1	0
3	A	715	OES	1	0
3	A	718	OES	1	0
3	A	719	OES	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	805:GLY	C	806:GLY	N	5.23
1	B	804:GLY	C	805:GLY	N	5.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	697/714 (97%)	-0.65	3 (0%) 88 86	32, 49, 78, 107	0
2	B	3/6 (50%)	-0.70	0 100 100	54, 54, 55, 57	0
All	All	700/720 (97%)	-0.65	3 (0%) 88 86	32, 49, 78, 107	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	TYR	2.7
1	A	219	PHE	2.3
1	A	576	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AHO	B	801	12/13	0.97	0.06	34,39,52,54	0
2	AHO	B	802	12/13	0.97	0.07	35,40,46,47	0
2	AHO	B	803	12/13	0.97	0.09	42,45,51,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OES	A	720	13/13	0.68	0.15	90,99,111,112	0
3	OES	A	717	13/13	0.69	0.16	85,91,99,100	0
3	OES	A	722	13/13	0.73	0.15	95,103,108,109	0
3	OES	A	721	13/13	0.76	0.14	93,102,110,111	0
3	OES	A	715	13/13	0.76	0.19	58,83,87,88	0
3	OES	A	718	13/13	0.78	0.13	91,97,106,107	0
3	OES	A	716	13/13	0.82	0.17	86,91,102,103	0
3	OES	A	719	13/13	0.83	0.14	87,89,97,99	0
4	FE	B	800	1/1	1.00	0.04	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.