



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:12 PM GMT

PDB ID : 3BEJ
Title : Structure of human FXR in complex with MFA-1 and co-activator peptide
Authors : Soisson, S.M.; Parthasarathy, G; Becker, J.W.
Deposited on : 2007-11-19
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

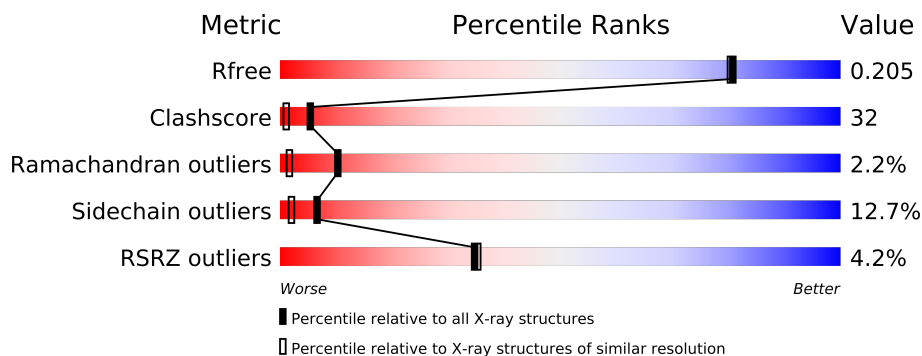
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	238	
1	B	238	
2	E	25	
2	F	25	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4349 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Bile acid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1842	1178	310	343	11			
1	B	228	Total	C	N	O	S	0	0	0
			1872	1197	314	350	11			

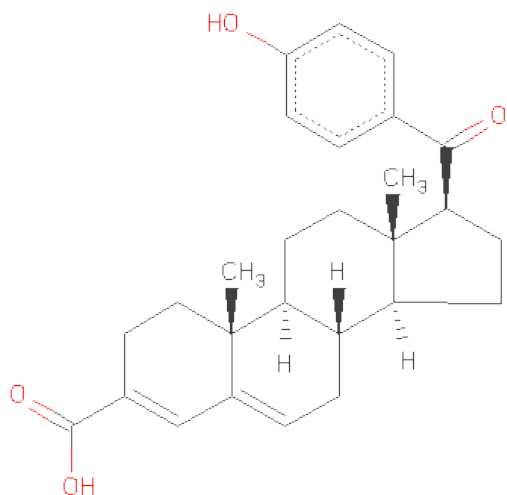
- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			101	64	23	14			
2	F	12	Total	C	N	O	0	0	0
			108	68	24	16			

- Molecule 3 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Y	0	0
			1	1		
3	A	1	Total	Y	0	0
			1	1		

- Molecule 4 is (8ALPHA,10ALPHA,13ALPHA,17BETA)-17-[(4-HYDROXYPHENYL)CARBONYL]ANDROSTA-3,5-DIENE-3-CARBOXYLICACID (three-letter code: MUF) (formula: C₂₇H₃₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			31	27	4		
4	B	1	Total	C	O	0	0
			31	27	4		

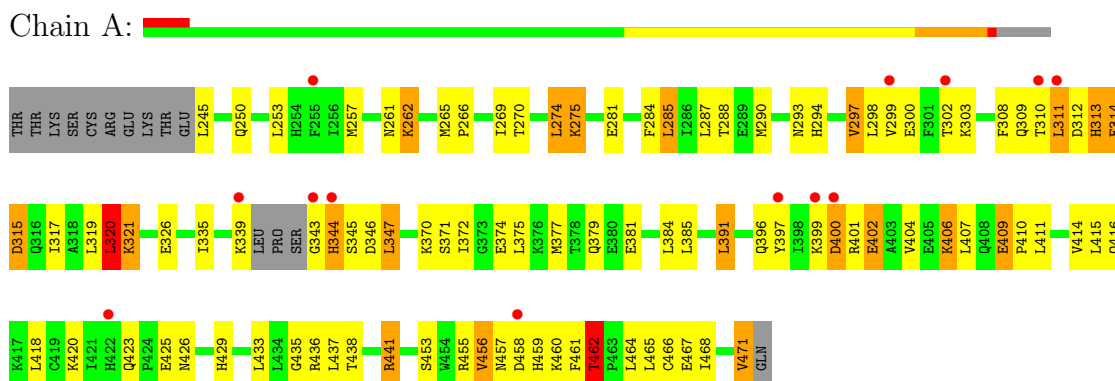
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		
5	B	213	Total	O	0	0
			213	213		
5	E	4	Total	O	0	0
			4	4		
5	F	4	Total	O	0	0
			4	4		

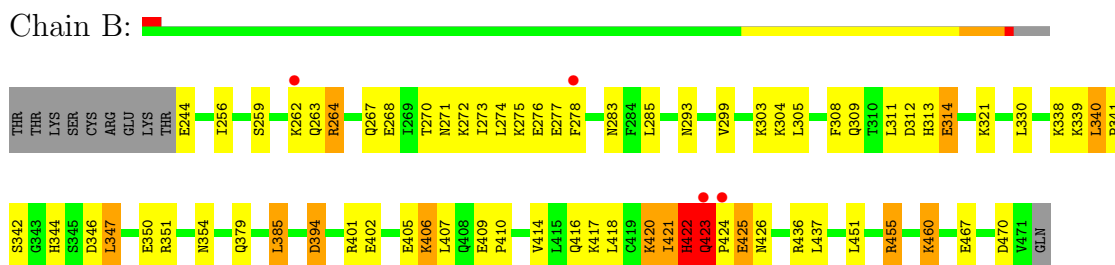
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

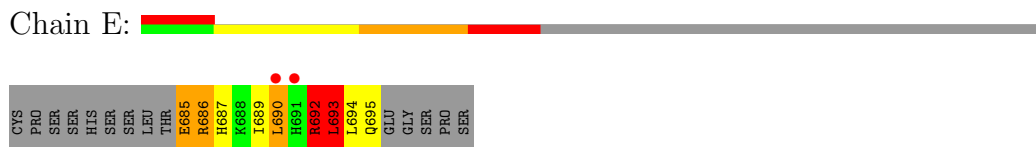
• Molecule 1: Bile acid receptor



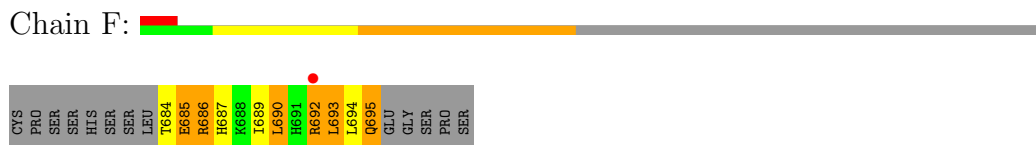
• Molecule 1: Bile acid receptor



• Molecule 2: Nuclear receptor coactivator 1



• Molecule 2: Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.64Å 90.89Å 129.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 1.90 39.65 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.65-1.90) 99.5 (39.65-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.89Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.200 , 0.254 0.207 , 0.205	Depositor DCC
R_{free} test set	3998 reflections (11.17%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39796 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4349	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MUF, YT3

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	0/1880	0.73	1/2537 (0.0%)
1	B	0.67	0/1912	0.78	1/2583 (0.0%)
2	E	0.37	0/102	0.89	0/134
2	F	0.47	0/109	1.01	0/144
All	All	0.61	0/4003	0.76	2/5398 (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	320	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	422	HIS	N-CA-C	5.25	125.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1838	132	0
1	B	1872	0	1868	96	0
2	E	101	0	110	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	108	0	117	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	30	1	0
4	B	31	0	31	0	0
5	A	141	0	0	17	0
5	B	213	0	0	9	0
5	E	4	0	0	1	0
5	F	4	0	0	2	0
All	All	4349	0	3994	259	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (259) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:LEU:HD12	1:A:437:LEU:HD21	1.22	1.14
2:E:685:GLU:HB3	2:E:687:HIS:HD1	1.05	1.12
1:A:266:PRO:HB2	1:A:269:ILE:HD13	1.25	1.10
1:B:385:LEU:HD11	1:B:437:LEU:HD21	1.32	1.06
1:B:423:GLN:HB2	1:B:424:PRO:HD3	1.39	1.05
1:A:317:ILE:HG21	2:E:685:GLU:HG3	1.37	1.03
2:E:685:GLU:HA	2:E:686:ARG:HB3	1.05	1.03
1:B:423:GLN:HB2	1:B:424:PRO:CD	1.92	0.97
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.31	0.95
2:E:685:GLU:HA	2:E:686:ARG:CB	1.96	0.95
2:E:685:GLU:CA	2:E:686:ARG:HB3	1.96	0.95
1:B:264:ARG:HH11	1:B:264:ARG:HG3	1.34	0.92
1:B:321:LYS:HZ3	2:F:687:HIS:CE1	1.87	0.91
1:B:321:LYS:HZ3	2:F:687:HIS:HE1	0.94	0.89
1:A:455:ARG:HH11	1:A:455:ARG:HG3	1.36	0.89
2:E:685:GLU:HB3	2:E:687:HIS:ND1	1.88	0.87
1:A:294:HIS:O	1:A:298:LEU:HD23	1.76	0.85
1:A:315:ASP:OD1	1:A:399:LYS:HG2	1.78	0.84
1:A:370:LYS:O	1:A:374:GLU:HG2	1.79	0.82
2:E:692:ARG:HE	2:E:693:LEU:N	1.77	0.82
1:B:385:LEU:HD11	1:B:437:LEU:CD2	2.11	0.81
1:A:414:VAL:O	1:A:418:LEU:HD13	1.80	0.81
1:A:467:GLU:OE1	2:E:689:ILE:HG22	1.80	0.81
1:B:385:LEU:CD1	1:B:437:LEU:HD21	2.10	0.80
1:A:294:HIS:NE2	1:A:298:LEU:HD21	1.96	0.80
1:A:315:ASP:OD2	1:A:400:ASP:HB2	1.82	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:ASP:OD2	1:A:347:LEU:HD13	1.81	0.80
1:A:344:HIS:HB2	5:A:547:HOH:O	1.82	0.78
1:A:423:GLN:HE22	1:A:426:ASN:HD22	1.30	0.78
1:A:423:GLN:HE21	1:A:426:ASN:HB3	1.48	0.78
1:A:429:HIS:O	1:A:433:LEU:HD23	1.82	0.78
1:A:402:GLU:O	1:A:406:LYS:HD3	1.84	0.78
1:B:270:THR:O	1:B:274:LEU:HD13	1.83	0.78
1:B:330:LEU:HD22	1:B:385:LEU:HD12	1.67	0.77
1:A:385:LEU:HD12	1:A:437:LEU:CD2	2.10	0.77
1:A:266:PRO:HB2	1:A:269:ILE:CD1	2.12	0.76
1:A:266:PRO:CB	1:A:269:ILE:HD13	2.09	0.76
1:B:385:LEU:HD13	1:B:385:LEU:O	1.87	0.75
1:A:294:HIS:CD2	1:A:298:LEU:HD21	2.24	0.73
1:A:310:THR:HB	5:A:560:HOH:O	1.88	0.72
1:A:321:LYS:HE3	2:E:687:HIS:NE2	2.03	0.72
1:B:421:ILE:N	1:B:421:ILE:HD13	2.04	0.72
1:A:344:HIS:NE2	5:A:536:HOH:O	2.21	0.71
1:A:455:ARG:NH1	1:A:455:ARG:HG3	2.03	0.71
1:B:455:ARG:HG3	1:B:455:ARG:NH1	2.06	0.70
1:A:300:GLU:HG2	5:A:569:HOH:O	1.91	0.70
1:A:312:ASP:O	1:A:314:GLU:N	2.24	0.70
1:B:259:SER:OG	1:B:304:LYS:HD3	1.92	0.69
1:A:245:LEU:N	5:A:581:HOH:O	2.24	0.69
1:A:344:HIS:N	1:A:346:ASP:OD1	2.26	0.69
1:B:422:HIS:ND1	1:B:423:GLN:HG3	2.09	0.68
1:B:308:PHE:O	1:B:311:LEU:HD23	1.94	0.68
1:B:414:VAL:O	1:B:418:LEU:HD13	1.92	0.68
1:B:311:LEU:HD21	1:B:407:LEU:HD11	1.74	0.68
1:B:405:GLU:O	1:B:409:GLU:HG3	1.94	0.68
1:B:264:ARG:NH1	1:B:264:ARG:HG3	2.07	0.67
2:E:685:GLU:OE2	2:E:685:GLU:N	2.27	0.67
1:A:467:GLU:CD	2:E:689:ILE:HG22	2.14	0.67
1:B:421:ILE:O	1:B:422:HIS:HB2	1.94	0.67
1:B:405:GLU:HB3	1:B:406:LYS:HE2	1.76	0.67
1:A:455:ARG:HD3	1:A:461:PHE:HE1	1.60	0.66
1:B:299:VAL:HG12	1:B:303:LYS:HD2	1.77	0.66
1:B:321:LYS:NZ	2:F:687:HIS:HE1	1.82	0.66
1:A:320:LEU:HD12	2:E:690:LEU:HD11	1.77	0.66
1:A:311:LEU:HD23	5:A:607:HOH:O	1.95	0.66
1:A:321:LYS:HA	1:A:468:ILE:HD11	1.78	0.66
1:B:424:PRO:O	1:B:425:GLU:HB2	1.96	0.66
1:B:314:GLU:HG2	5:B:750:HOH:O	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:MET:HE1	1:A:290:MET:HE2	1.78	0.64
1:B:460:LYS:NZ	5:B:641:HOH:O	2.30	0.64
1:B:330:LEU:CD2	1:B:385:LEU:HD12	2.27	0.64
1:A:315:ASP:CG	1:A:399:LYS:HG2	2.18	0.64
1:A:429:HIS:CE1	1:A:433:LEU:HD21	2.32	0.64
1:A:385:LEU:HD21	1:A:415:LEU:HD21	1.80	0.63
2:F:693:LEU:HD12	2:F:694:LEU:N	2.12	0.63
1:A:379:GLN:HG2	5:A:548:HOH:O	1.99	0.63
1:A:453:SER:O	1:A:456:VAL:HG12	1.99	0.63
2:E:692:ARG:HH21	2:E:693:LEU:HA	1.64	0.63
1:B:338:LYS:O	1:B:344:HIS:HE1	1.82	0.62
1:B:311:LEU:N	1:B:311:LEU:HD22	2.15	0.62
1:A:399:LYS:HG3	1:A:400:ASP:N	2.16	0.61
2:F:690:LEU:HD23	2:F:693:LEU:HD11	1.81	0.61
2:F:685:GLU:HA	2:F:687:HIS:H	1.66	0.60
1:A:399:LYS:HG3	1:A:400:ASP:H	1.65	0.60
1:A:423:GLN:HE22	1:A:426:ASN:ND2	1.97	0.60
2:E:692:ARG:HE	2:E:693:LEU:CA	2.14	0.60
1:B:455:ARG:HA	1:B:455:ARG:NE	2.16	0.60
1:A:372:ILE:HD13	1:A:436:ARG:HG2	1.84	0.59
1:B:421:ILE:O	1:B:422:HIS:CB	2.50	0.59
1:B:402:GLU:OE2	1:B:406:LYS:NZ	2.29	0.59
1:B:278:PHE:HE2	1:B:354:ASN:HD22	1.47	0.59
1:B:423:GLN:CB	1:B:424:PRO:CD	2.77	0.59
1:B:293:ASN:HB2	5:B:649:HOH:O	2.02	0.59
1:B:385:LEU:HD21	1:B:437:LEU:HD21	1.85	0.58
1:B:268:GLU:O	1:B:272:LYS:HG3	2.02	0.58
1:A:437:LEU:O	1:A:441:ARG:HG2	2.03	0.58
1:A:284:PHE:CE2	1:A:459:HIS:HB3	2.38	0.58
2:F:694:LEU:O	2:F:695:GLN:HB2	2.03	0.58
1:A:269:ILE:HD12	1:A:269:ILE:N	2.18	0.58
1:B:455:ARG:CG	1:B:455:ARG:HH11	2.12	0.57
1:A:313:HIS:HD2	5:A:599:HOH:O	1.87	0.57
2:E:693:LEU:HD12	2:E:693:LEU:N	2.20	0.57
1:B:425:GLU:OE2	1:B:425:GLU:HA	2.03	0.57
1:B:402:GLU:HG3	1:B:406:LYS:HE3	1.85	0.57
1:B:421:ILE:HG22	1:B:422:HIS:N	2.18	0.56
1:A:401:ARG:HD3	5:A:612:HOH:O	2.04	0.56
2:E:685:GLU:CB	2:E:687:HIS:H	2.19	0.56
1:A:399:LYS:CG	1:A:400:ASP:H	2.19	0.56
1:A:281:GLU:O	1:A:285:LEU:HD13	2.06	0.56
1:B:340:LEU:HD12	1:B:340:LEU:N	2.20	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:299:VAL:HG21	2:F:693:LEU:HD13	1.89	0.55
1:A:294:HIS:CD2	1:A:298:LEU:CD2	2.89	0.55
1:B:299:VAL:CG1	1:B:303:LYS:HD2	2.37	0.55
1:B:405:GLU:HG2	1:B:409:GLU:OE2	2.07	0.54
1:A:326:GLU:OE2	1:A:441:ARG:NH1	2.41	0.54
1:A:298:LEU:HD22	1:A:298:LEU:N	2.22	0.53
1:A:455:ARG:HD3	1:A:461:PHE:CE1	2.40	0.53
1:A:314:GLU:HG3	5:E:327:HOH:O	2.06	0.53
1:A:339:LYS:O	1:A:343:GLY:O	2.26	0.53
1:A:262:LYS:HG3	1:A:262:LYS:O	2.08	0.53
1:B:303:LYS:O	1:B:309:GLN:OE1	2.25	0.53
2:F:685:GLU:CA	2:F:687:HIS:H	2.21	0.53
2:F:685:GLU:HA	2:F:687:HIS:N	2.24	0.53
1:B:273:ILE:O	1:B:347:LEU:HD12	2.09	0.53
1:A:308:PHE:O	1:A:311:LEU:HB2	2.09	0.53
1:B:276:GLU:HG3	1:B:277:GLU:N	2.23	0.52
1:B:379:GLN:HG2	5:B:681:HOH:O	2.09	0.52
1:A:343:GLY:O	1:A:345:SER:N	2.35	0.52
1:B:385:LEU:HD13	1:B:385:LEU:C	2.29	0.52
1:A:462:THR:HG22	1:A:465:LEU:H	1.72	0.52
1:A:384:LEU:CD1	1:A:418:LEU:HD22	2.40	0.52
1:B:271:ASN:O	1:B:275:LYS:HG2	2.10	0.52
1:B:418:LEU:HD12	1:B:418:LEU:N	2.24	0.52
1:A:396:GLN:HG2	1:A:397:TYR:CD2	2.45	0.52
2:E:692:ARG:HE	2:E:693:LEU:HA	1.74	0.51
1:A:466:CYS:HA	1:A:471:VAL:HG13	1.92	0.51
1:B:421:ILE:HD11	5:B:710:HOH:O	2.11	0.51
1:A:441:ARG:NE	5:A:526:HOH:O	2.33	0.51
1:A:311:LEU:HD12	1:A:407:LEU:HD11	1.93	0.51
1:A:287:LEU:HB3	4:A:473:MUF:H53	1.93	0.51
1:B:313:HIS:HD2	5:F:229:HOH:O	1.93	0.50
1:A:385:LEU:CD2	1:A:415:LEU:HD21	2.41	0.50
1:A:375:LEU:HD11	1:A:436:ARG:HD3	1.94	0.50
1:B:385:LEU:HD21	1:B:437:LEU:CG	2.41	0.49
1:B:256:ILE:HD12	1:B:305:LEU:HD23	1.94	0.49
1:B:394:ASP:HA	1:B:401:ARG:NH1	2.27	0.49
1:A:303:LYS:HZ1	2:E:695:GLN:N	2.10	0.49
1:A:416:GLN:NE2	5:A:529:HOH:O	2.46	0.49
1:A:399:LYS:CG	1:A:400:ASP:N	2.75	0.49
1:B:467:GLU:OE2	2:F:689:ILE:HG13	2.12	0.49
1:A:245:LEU:N	5:A:539:HOH:O	2.45	0.49
1:A:298:LEU:CD2	1:A:298:LEU:N	2.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:256:ILE:HD12	1:B:305:LEU:CD2	2.42	0.49
2:F:690:LEU:O	2:F:693:LEU:HD12	2.12	0.48
1:A:409:GLU:HB3	1:A:410:PRO:HD3	1.96	0.48
1:A:288:THR:HG21	1:A:461:PHE:O	2.13	0.48
2:E:692:ARG:O	2:E:694:LEU:N	2.47	0.48
1:A:320:LEU:HD12	2:E:690:LEU:HD21	1.96	0.48
2:E:692:ARG:NE	2:E:693:LEU:N	2.55	0.47
1:B:244:GLU:N	5:B:742:HOH:O	2.47	0.47
2:F:692:ARG:HG3	2:F:692:ARG:HH11	1.78	0.47
1:A:311:LEU:HD12	1:A:407:LEU:CD1	2.45	0.47
1:B:385:LEU:HD21	1:B:437:LEU:CD2	2.44	0.47
1:B:421:ILE:N	1:B:421:ILE:CD1	2.73	0.47
1:A:423:GLN:NE2	1:A:426:ASN:HB3	2.22	0.47
1:B:347:LEU:HD13	1:B:351:ARG:NE	2.30	0.47
1:A:269:ILE:HG21	1:A:290:MET:HG2	1.97	0.47
1:A:317:ILE:CG2	2:E:685:GLU:HG3	2.26	0.47
1:B:407:LEU:O	1:B:410:PRO:HD2	2.14	0.47
1:B:341:PRO:O	1:B:344:HIS:HB3	2.15	0.46
1:B:299:VAL:HG11	2:F:693:LEU:HD13	1.97	0.46
2:E:692:ARG:NH2	2:E:693:LEU:HA	2.30	0.46
2:F:693:LEU:HD12	2:F:693:LEU:C	2.36	0.46
1:A:391:LEU:CD2	1:A:411:LEU:HD11	2.45	0.46
1:A:321:LYS:HA	1:A:468:ILE:CD1	2.43	0.46
1:A:423:GLN:NE2	1:A:426:ASN:HD22	2.06	0.46
1:B:385:LEU:CD2	1:B:437:LEU:HD21	2.46	0.46
1:A:344:HIS:HD2	5:A:616:HOH:O	1.99	0.46
1:B:273:ILE:O	1:B:351:ARG:NH2	2.42	0.46
1:B:422:HIS:ND1	1:B:423:GLN:CG	2.78	0.46
1:B:338:LYS:O	1:B:344:HIS:CE1	2.65	0.46
1:B:417:LYS:HE3	5:B:717:HOH:O	2.15	0.46
2:E:690:LEU:HA	2:E:693:LEU:HD11	1.98	0.46
1:A:343:GLY:HA3	1:A:346:ASP:OD1	2.17	0.46
1:A:302:THR:HG22	1:A:308:PHE:CE2	2.51	0.45
2:E:689:ILE:CG2	2:E:690:LEU:N	2.79	0.45
1:A:299:VAL:CG2	1:A:320:LEU:HD11	2.46	0.45
1:A:343:GLY:O	1:A:344:HIS:HB3	2.16	0.45
1:A:311:LEU:CD1	1:A:407:LEU:CD1	2.94	0.45
2:F:684:THR:HB	5:F:183:HOH:O	2.17	0.45
1:A:250:GLN:HG2	5:A:582:HOH:O	2.17	0.45
1:A:375:LEU:HD11	1:A:436:ARG:CD	2.47	0.45
1:A:377:MET:HA	1:A:381:GLU:OE1	2.17	0.45
1:A:321:LYS:CE	2:E:687:HIS:NE2	2.76	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:ARG:CG	1:B:264:ARG:NH1	2.72	0.45
1:A:385:LEU:HD22	1:A:415:LEU:HD22	1.99	0.45
1:A:455:ARG:CD	1:A:461:PHE:HE1	2.27	0.45
2:E:689:ILE:HG23	2:E:690:LEU:N	2.31	0.45
1:A:257:MET:O	1:A:261:ASN:HB2	2.17	0.45
1:A:274:LEU:HB3	1:A:275:LYS:HG2	1.99	0.45
1:A:293:ASN:O	1:A:297:VAL:HG13	2.17	0.45
1:B:455:ARG:CG	1:B:455:ARG:NH1	2.74	0.45
1:A:409:GLU:HB3	1:A:410:PRO:CD	2.47	0.45
1:B:283:ASN:OD1	1:B:351:ARG:HG2	2.17	0.44
1:A:270:THR:HG23	1:A:344:HIS:NE2	2.31	0.44
1:B:340:LEU:HB3	1:B:341:PRO:HA	1.99	0.44
1:A:455:ARG:HA	1:A:455:ARG:HD2	1.63	0.44
1:A:321:LYS:HA	1:A:468:ILE:CG1	2.47	0.44
1:B:424:PRO:HB2	5:B:685:HOH:O	2.18	0.44
1:A:423:GLN:NE2	1:A:426:ASN:CB	2.80	0.44
1:A:371:SER:O	1:A:436:ARG:NH2	2.47	0.44
1:A:321:LYS:HE3	2:E:687:HIS:CD2	2.52	0.44
1:B:423:GLN:OE1	1:B:424:PRO:HD2	2.17	0.44
1:B:424:PRO:O	1:B:425:GLU:CB	2.64	0.44
1:A:343:GLY:C	1:A:345:SER:H	2.18	0.44
1:A:381:GLU:OE2	1:A:429:HIS:HE1	2.00	0.44
1:A:265:MET:HE2	5:A:570:HOH:O	2.17	0.44
1:B:385:LEU:HD21	1:B:437:LEU:HG	1.99	0.44
1:B:423:GLN:CD	1:B:424:PRO:HD2	2.38	0.44
1:A:303:LYS:HZ1	2:E:695:GLN:HB2	1.83	0.43
1:A:436:ARG:HD2	5:A:530:HOH:O	2.17	0.43
1:B:299:VAL:HG21	2:F:693:LEU:CD1	2.49	0.43
2:E:685:GLU:HB2	2:E:687:HIS:H	1.82	0.43
1:A:269:ILE:HD12	1:A:269:ILE:H	1.84	0.43
1:A:423:GLN:HE21	1:A:426:ASN:CB	2.23	0.43
2:F:690:LEU:CD2	2:F:693:LEU:HD11	2.49	0.43
1:A:317:ILE:O	1:A:321:LYS:HB3	2.19	0.43
1:B:274:LEU:N	1:B:274:LEU:CD1	2.82	0.43
1:A:460:LYS:HE3	1:A:460:LYS:HB3	1.36	0.43
1:A:265:MET:CE	1:A:290:MET:HE2	2.47	0.43
1:A:409:GLU:CB	1:A:410:PRO:CD	2.97	0.43
1:B:346:ASP:O	1:B:350:GLU:HG2	2.19	0.42
1:B:299:VAL:HG12	1:B:303:LYS:CD	2.49	0.42
1:A:423:GLN:HB3	1:A:423:GLN:HE21	1.54	0.42
1:A:339:LYS:HB2	5:A:540:HOH:O	2.20	0.42
1:B:436:ARG:HD3	1:B:436:ARG:HA	1.77	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:LEU:O	1:A:257:MET:HG2	2.20	0.42
2:F:684:THR:O	2:F:686:ARG:HB2	2.20	0.42
1:A:265:MET:CE	1:A:290:MET:CE	2.98	0.41
1:B:308:PHE:HA	1:B:311:LEU:HD23	2.01	0.41
1:B:347:LEU:HA	1:B:347:LEU:HD23	1.74	0.41
1:A:319:LEU:HD21	1:A:404:VAL:HG11	2.02	0.41
1:A:381:GLU:O	1:A:385:LEU:HD23	2.20	0.41
1:A:245:LEU:HD21	1:A:418:LEU:CD1	2.51	0.41
1:B:406:LYS:HD3	1:B:406:LYS:HA	1.60	0.41
1:B:340:LEU:HA	1:B:341:PRO:C	2.40	0.41
1:B:416:GLN:O	1:B:420:LYS:HD2	2.20	0.41
1:B:263:GLN:OE1	1:B:263:GLN:N	2.48	0.41
1:B:311:LEU:N	1:B:311:LEU:CD2	2.81	0.41
1:A:385:LEU:CD2	1:A:415:LEU:CD2	2.98	0.41
1:A:461:PHE:O	1:A:462:THR:CB	2.69	0.41
1:A:270:THR:HG23	1:A:344:HIS:CE1	2.56	0.41
1:A:311:LEU:CD1	1:A:407:LEU:HD12	2.50	0.41
1:A:265:MET:HE1	1:A:290:MET:CE	2.50	0.40
1:A:456:VAL:CG1	1:A:457:ASN:N	2.84	0.40
1:B:426:ASN:N	5:B:685:HOH:O	2.46	0.40
1:A:435:GLY:O	1:A:438:THR:HB	2.22	0.40
1:B:311:LEU:HD21	1:B:407:LEU:CD1	2.47	0.40
1:A:418:LEU:N	1:A:418:LEU:HD12	2.37	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	220/238 (92%)	207 (94%)	9 (4%)	4 (2%)	13	3
1	B	226/238 (95%)	216 (96%)	7 (3%)	3 (1%)	18	5
2	E	9/25 (36%)	5 (56%)	1 (11%)	3 (33%)	0	0
2	F	10/25 (40%)	7 (70%)	3 (30%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	465/526 (88%)	435 (94%)	20 (4%)	10 (2%)	10	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	B	423	GLN
1	B	425	GLU
2	E	692	ARG
2	E	686	ARG
2	E	693	LEU
1	A	309	GLN
1	A	314	GLU
1	A	462	THR
1	B	422	HIS

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	207/221 (94%)	182 (88%)	25 (12%)	7	2
1	B	211/221 (96%)	190 (90%)	21 (10%)	11	4
2	E	11/24 (46%)	7 (64%)	4 (36%)	0	0
2	F	12/24 (50%)	6 (50%)	6 (50%)	0	0
All	All	441/490 (90%)	385 (87%)	56 (13%)	6	2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	LYS
1	A	274	LEU
1	A	275	LYS
1	A	285	LEU
1	A	297	VAL
1	A	311	LEU

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Mol	Chain	Res	Type
1	A	315	ASP
1	A	320	LEU
1	A	321	LYS
1	A	335	ILE
1	A	344	HIS
1	A	347	LEU
1	A	391	LEU
1	A	400	ASP
1	A	402	GLU
1	A	406	LYS
1	A	409	GLU
1	A	420	LYS
1	A	425	GLU
1	A	441	ARG
1	A	456	VAL
1	A	458	ASP
1	A	462	THR
1	A	464	LEU
1	A	471	VAL
1	B	262	LYS
1	B	264	ARG
1	B	267	GLN
1	B	285	LEU
1	B	312	ASP
1	B	314	GLU
1	B	339	LYS
1	B	340	LEU
1	B	342	SER
1	B	347	LEU
1	B	385	LEU
1	B	394	ASP
1	B	406	LYS
1	B	420	LYS
1	B	421	ILE
1	B	422	HIS
1	B	423	GLN
1	B	451	LEU
1	B	455	ARG
1	B	460	LYS
1	B	470	ASP
2	E	685	GLU
2	E	690	LEU

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Mol	Chain	Res	Type
2	E	692	ARG
2	E	693	LEU
2	F	685	GLU
2	F	686	ARG
2	F	690	LEU
2	F	692	ARG
2	F	693	LEU
2	F	695	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	423	GLN
1	A	429	HIS
1	A	457	ASN
1	A	459	HIS
1	B	250	GLN
1	B	267	GLN
1	B	344	HIS
1	B	379	GLN
2	E	695	GLN
2	F	687	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	MUF	A	473	-	35,35,35	1.76	12 (34%)	55,55,55	1.97	14 (25%)
4	MUF	B	1	-	35,35,35	1.67	8 (22%)	55,55,55	2.02	15 (27%)

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	MUF	A	473	-	-	0/12/70/70	0/1/5/5
4	MUF	B	1	-	-	0/12/70/70	0/1/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	MUF	O76-C28	4.21	1.35	1.22
4	A	473	MUF	O76-C28	3.99	1.34	1.22
4	B	1	MUF	C1-C10	2.87	1.59	1.54
4	A	473	MUF	C1-C10	2.77	1.59	1.54
4	A	473	MUF	C19-C10	2.60	1.59	1.54
4	A	473	MUF	C6-C5	2.56	1.36	1.33
4	A	473	MUF	C7-C8	2.51	1.58	1.53
4	A	473	MUF	O82-C28	-2.49	1.22	1.30
4	A	473	MUF	C12-C13	2.48	1.58	1.54
4	B	1	MUF	C12-C13	2.46	1.58	1.54
4	A	473	MUF	C10-C5	2.43	1.56	1.52
4	B	1	MUF	O82-C28	-2.40	1.22	1.30
4	B	1	MUF	C6-C5	2.34	1.36	1.33
4	A	473	MUF	C18-C13	2.30	1.58	1.54
4	A	473	MUF	C53-C52	2.28	1.43	1.39
4	B	1	MUF	C57-C52	2.23	1.43	1.39
4	A	473	MUF	C10-C9	2.22	1.60	1.56
4	B	1	MUF	C19-C10	2.16	1.58	1.54
4	B	1	MUF	C7-C8	2.12	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	473	MUF	C57-C52	2.06	1.42	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	473	MUF	C13-C17-C20	-6.78	106.86	115.17
4	B	1	MUF	C13-C17-C20	-6.25	107.51	115.17
4	B	1	MUF	O76-C28-C3	-5.70	111.34	121.28
4	A	473	MUF	O76-C28-C3	-5.61	111.50	121.28
4	A	473	MUF	C16-C17-C13	-4.08	99.92	104.14
4	A	473	MUF	O82-C28-C3	3.82	124.75	115.63
4	B	1	MUF	O82-C28-C3	3.81	124.72	115.63
4	B	1	MUF	C1-C10-C5	-3.57	105.24	108.78
4	B	1	MUF	C16-C17-C20	3.31	120.10	112.08
4	A	473	MUF	C16-C17-C20	3.25	119.96	112.08
4	B	1	MUF	C9-C10-C5	3.24	112.31	108.02
4	B	1	MUF	C12-C13-C17	3.10	119.38	116.20
4	A	473	MUF	C4-C3-C28	-3.04	114.67	120.95
4	B	1	MUF	C18-C13-C12	-2.89	105.77	110.55
4	A	473	MUF	C8-C7-C6	2.77	117.47	112.84
4	A	473	MUF	C2-C3-C28	2.63	122.23	117.19
4	B	1	MUF	C8-C7-C6	2.63	117.24	112.84
4	B	1	MUF	C17-C13-C14	-2.59	96.94	99.68
4	B	1	MUF	C12-C11-C9	-2.47	109.02	113.15
4	A	473	MUF	C17-C13-C14	-2.37	97.16	99.68
4	B	1	MUF	C4-C3-C28	-2.37	116.05	120.95
4	B	1	MUF	C2-C3-C28	2.35	121.69	117.19
4	B	1	MUF	C18-C13-C14	2.30	116.35	111.76
4	A	473	MUF	C18-C13-C12	-2.30	106.75	110.55
4	A	473	MUF	C1-C10-C5	-2.24	106.55	108.78
4	A	473	MUF	O52-C20-C52	-2.21	117.47	120.54
4	B	1	MUF	C54-C53-C52	-2.19	118.14	120.76
4	A	473	MUF	C12-C13-C17	2.19	118.44	116.20
4	A	473	MUF	C18-C13-C17	2.04	113.18	110.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	224/238 (94%)	0.31	13 (5%) 22 22	16, 35, 61, 75	0
1	B	228/238 (95%)	0.03	4 (1%) 65 67	16, 25, 50, 78	0
2	E	11/25 (44%)	1.22	2 (18%) 2 2	46, 52, 67, 69	0
2	F	12/25 (48%)	0.59	1 (8%) 11 11	30, 39, 62, 70	0
All	All	475/526 (90%)	0.21	20 (4%) 35 35	16, 31, 61, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	GLY	9.4
1	B	424	PRO	7.2
1	B	423	GLN	6.5
1	A	344	HIS	4.7
1	A	400	ASP	4.3
1	A	458	ASP	3.2
1	A	399	LYS	3.2
1	A	397	TYR	3.0
1	B	278	PHE	2.8
1	B	262	LYS	2.6
1	A	311	LEU	2.5
1	A	422	HIS	2.4
1	A	310	THR	2.3
2	E	690	LEU	2.3
1	A	302	THR	2.2
1	A	339	LYS	2.2
2	E	691	HIS	2.2
2	F	692	ARG	2.1
1	A	255	PHE	2.1
1	A	299	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	YT3	B	2	1/1	0.09	0.25	18,18,18,18	0
4	MUF	B	1	31/31	0.09	-0.37	12,20,26,32	0
4	MUF	A	473	31/31	0.10	-0.46	20,28,37,38	0
3	YT3	A	1	1/1	0.08	-2.54	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.