



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:22 AM UTC

PDB ID : 1XMC / pdb_00001xmc
Title : C323M mutant structure of mouse carnitine octanoyltransferase
Authors : Jogl, G.; Hsiao, Y.S.; Tong, L.
Deposited on : 2004-10-01
Resolution : 2.00 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

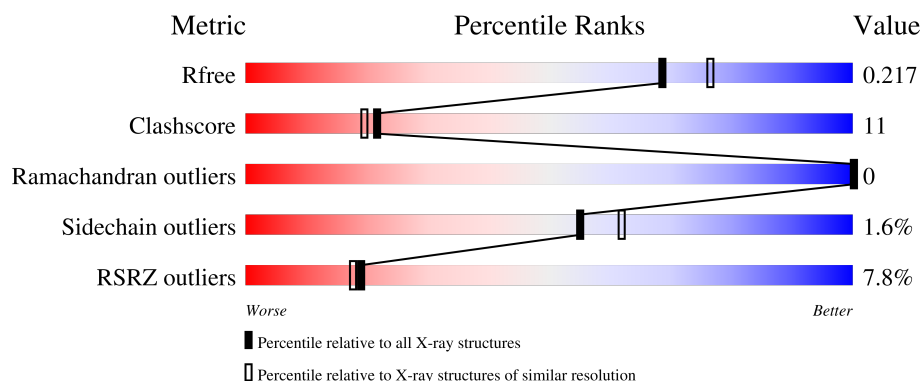
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	612	10% 74% 22% ..
1	B	612	5% 77% 19% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10264 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.

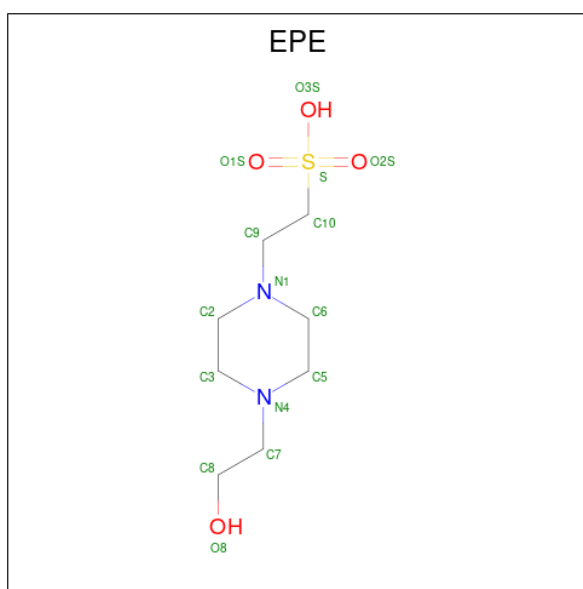
- Molecule 1 is a protein called Peroxisomal carnitine O-octanoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4778	3044	829	872	33			
1	B	600	Total	C	N	O	S	0	0	0
			4845	3087	839	886	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	MET	CYS	engineered mutation	UNP Q9DC50
B	323	MET	CYS	engineered mutation	UNP Q9DC50

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



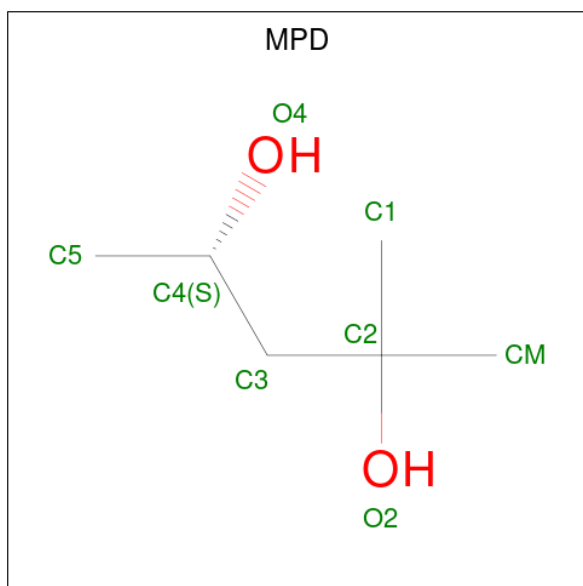
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total	O	0	0
			216	216		

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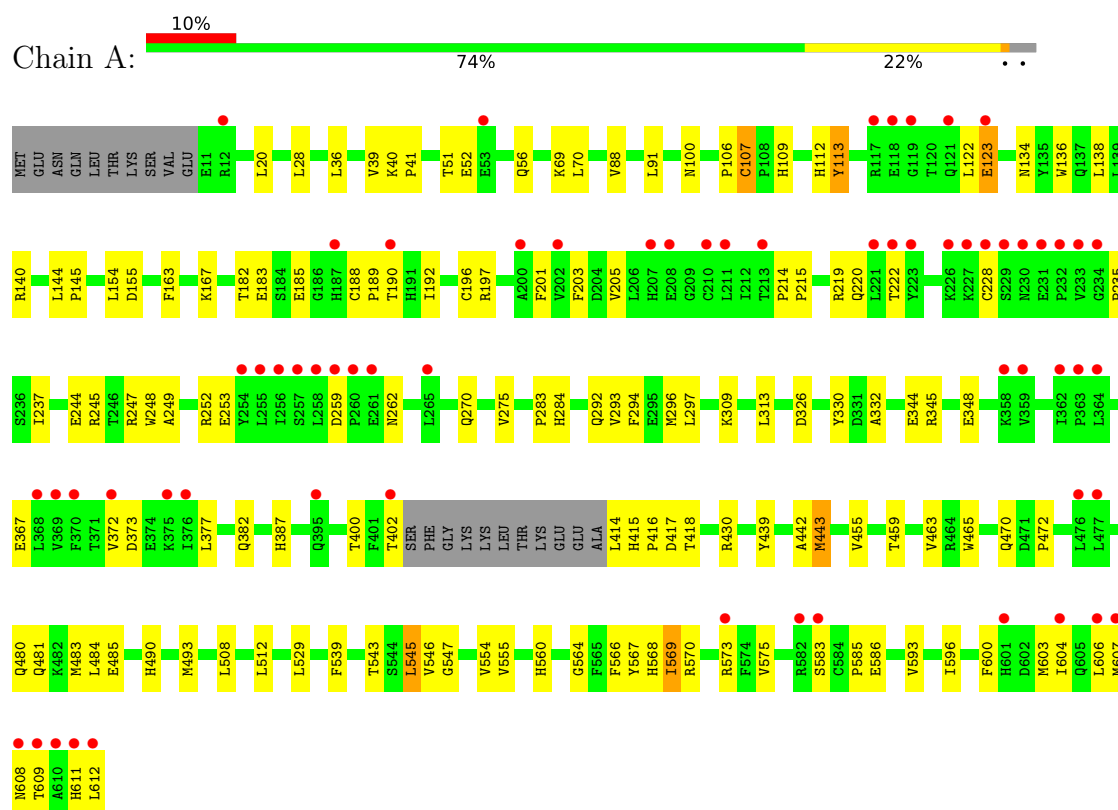
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	339	Total 339	O 339	0	0

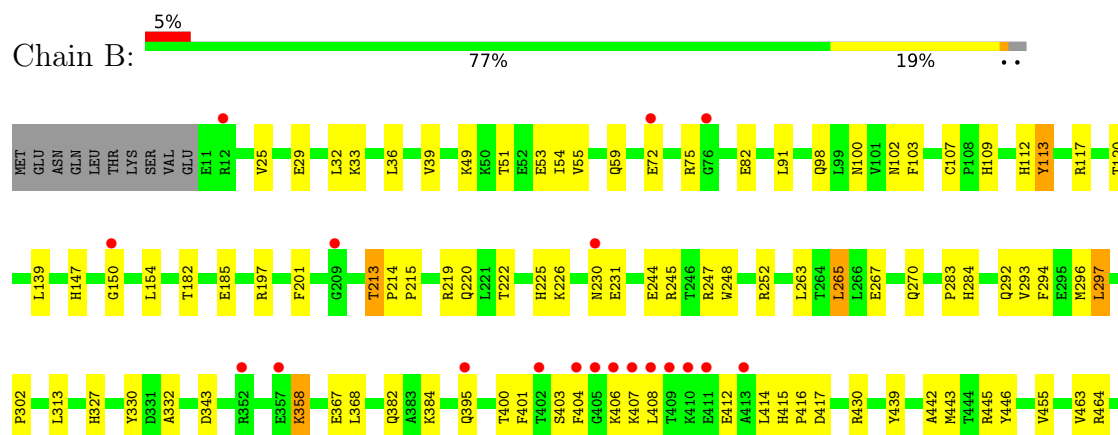
3 Residue-property plots

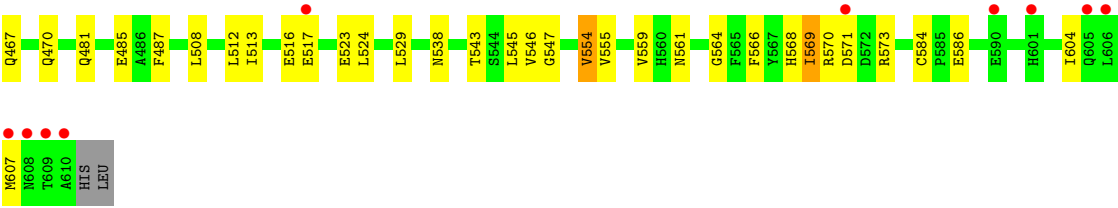
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Peroxisomal carnitine O-octanoyltransferase



- Molecule 1: Peroxisomal carnitine O-octanoyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	163.90Å 163.90Å 159.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.75 – 2.00 26.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (26.75-2.00) 90.3 (26.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.217 0.190 , 0.217	Depositor DCC
R_{free} test set	7313 reflections (7.36%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10264	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: EPE, MPD

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	0.34	0/4903	0.88	14/6638 (0.2%)
1	B	0.39	0/4971	0.89	20/6729 (0.3%)
All	All	0.37	0/9874	0.88	34/13367 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	564	GLY	N-CA-C	-8.66	97.46	110.71
1	B	332	ALA	N-CA-C	7.60	120.45	111.71
1	B	244	GLU	N-CA-C	-7.20	99.79	110.23
1	B	107	CYS	N-CA-C	-7.06	98.97	109.42
1	A	332	ALA	N-CA-C	6.99	120.91	112.38
1	B	245	ARG	N-CA-C	6.89	118.79	111.28
1	B	91	LEU	N-CA-C	6.48	119.17	111.71
1	B	545	LEU	N-CA-C	-6.43	100.05	110.20
1	B	113	TYR	N-CA-C	6.19	120.10	112.54
1	B	100	ASN	N-CA-C	6.18	120.66	113.18
1	B	543	THR	N-CA-C	6.16	118.31	109.14
1	A	543	THR	N-CA-C	5.93	117.97	109.14
1	B	213	THR	N-CA-C	5.92	116.93	110.13
1	A	244	GLU	N-CA-C	-5.90	101.68	110.23
1	A	100	ASN	N-CA-C	5.89	120.47	113.28
1	B	547	GLY	N-CA-C	5.85	119.18	111.52
1	B	150	GLY	N-CA-C	-5.85	99.33	113.18
1	B	446	TYR	N-CA-C	-5.84	105.04	111.82
1	A	91	LEU	N-CA-C	5.84	118.43	111.71
1	A	564	GLY	N-CA-C	-5.83	99.35	113.18
1	A	569	ILE	N-CA-C	5.62	115.97	108.11
1	A	245	ARG	N-CA-C	5.53	117.75	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	CYS	N-CA-C	-5.47	101.63	109.24
1	B	569	ILE	N-CA-C	5.46	115.75	108.11
1	B	25	VAL	N-CA-C	-5.30	101.69	107.73
1	A	113	TYR	N-CA-C	5.23	118.92	112.54
1	A	88	VAL	N-CA-C	5.22	115.99	110.72
1	A	107	CYS	CA-C-N	5.20	126.34	119.84
1	A	107	CYS	C-N-CA	5.20	126.34	119.84
1	B	82	GLU	N-CA-C	5.20	119.90	111.37
1	B	586	GLU	N-CA-C	5.19	116.63	111.07
1	A	545	LEU	N-CA-C	-5.17	102.03	110.20
1	B	107	CYS	CA-C-N	5.06	126.17	119.84
1	B	107	CYS	C-N-CA	5.06	126.17	119.84

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	4778	0	4680	100	0
1	B	4845	0	4754	105	0
2	A	15	0	18	0	0
2	B	15	0	18	2	0
3	A	8	0	14	0	0
3	B	48	0	84	9	0
4	A	216	0	0	3	0
4	B	339	0	0	9	0
All	All	10264	0	9568	208	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 11.

All (208) 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)
2:B:701:EPE:H101	3:B:702:MPD:H51	1.47	0.96
1:A:283:PRO:HA	1:A:292:GLN:HE21	1.32	0.95
1:A:219:ARG:HH21	1:A:220:GLN:HE22	1.11	0.94
1:B:284:HIS:H	1:B:292:GLN:NE2	1.71	0.89
1:B:252:ARG:HH21	1:B:270:GLN:HE22	1.24	0.83
1:A:568:HIS:HE1	1:A:570:ARG:HE	1.27	0.82
1:B:36:LEU:HD21	1:B:55:VAL:HG21	1.61	0.81
1:B:604:ILE:HA	1:B:607:MET:HE3	1.62	0.81
1:A:430:ARG:HE	1:A:470:GLN:HE22	1.29	0.80
1:A:483:MET:HE3	1:A:606:LEU:HD23	1.61	0.79
1:B:219:ARG:HH21	1:B:220:GLN:HE22	1.27	0.78
1:A:465:TRP:CZ2	1:A:483:MET:HE2	2.19	0.78
1:A:416:PRO:HB2	1:A:569:ILE:HD13	1.65	0.76
1:A:430:ARG:HE	1:A:470:GLN:NE2	1.83	0.76
1:A:252:ARG:HH21	1:A:270:GLN:HE22	1.33	0.75
1:B:36:LEU:HD21	1:B:55:VAL:HG11	1.69	0.75
1:A:123:GLU:CD	1:A:123:GLU:H	1.94	0.73
1:A:604:ILE:HA	1:A:607:MET:HE3	1.73	0.70
1:B:283:PRO:HA	1:B:292:GLN:HE21	1.55	0.70
1:B:430:ARG:HE	1:B:470:GLN:HE22	1.37	0.69
1:B:404:PHE:CZ	1:B:604:ILE:HG13	2.27	0.69
1:B:112:HIS:CD2	1:B:113:TYR:H	2.11	0.68
1:B:154:LEU:HD13	1:B:443:MET:HE1	1.73	0.68
1:B:443:MET:HE2	1:B:445:ARG:HD3	1.76	0.67
1:A:219:ARG:HH21	1:A:220:GLN:NE2	1.88	0.67
1:B:568:HIS:HE1	1:B:570:ARG:HE	1.42	0.67
1:A:465:TRP:HZ2	1:A:483:MET:HE2	1.59	0.66
1:B:284:HIS:H	1:B:292:GLN:HE21	1.43	0.66
1:A:182:THR:OG1	1:A:185:GLU:HG3	1.96	0.66
1:A:249:ALA:O	1:A:253:GLU:HG3	1.96	0.65
1:B:430:ARG:HE	1:B:470:GLN:NE2	1.93	0.65
1:B:538:ASN:HA	1:B:559:VAL:HG11	1.78	0.64
1:A:52:GLU:O	1:A:56:GLN:HG3	1.98	0.64
1:A:214:PRO:HB2	1:A:215:PRO:HD3	1.80	0.63
3:B:705:MPD:H51	4:B:840:HOH:O	1.99	0.63
1:A:112:HIS:CD2	1:A:113:TYR:H	2.16	0.63
1:A:167:LYS:HE3	1:A:326:ASP:OD2	1.98	0.63
1:A:283:PRO:HA	1:A:292:GLN:NE2	2.09	0.63
1:B:358:LYS:NZ	1:B:358:LYS:HB3	2.14	0.63
1:A:134:ASN:O	1:A:138:LEU:HD13	1.99	0.62
1:B:32:LEU:O	1:B:36:LEU:HD23	2.00	0.62
1:A:546:VAL:HG23	1:A:568:HIS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ARG:HD2	1:A:573:ARG:HH11	1.65	0.61
1:B:36:LEU:CD2	1:B:55:VAL:HG11	2.29	0.61
1:B:219:ARG:HH21	1:B:220:GLN:NE2	1.97	0.61
1:B:36:LEU:CD2	1:B:55:VAL:HG21	2.29	0.60
1:A:345:ARG:HH21	1:A:348:GLU:CD	2.10	0.59
1:A:344:GLU:O	1:A:348:GLU:HG3	2.02	0.59
1:A:568:HIS:CE1	1:A:570:ARG:HE	2.16	0.59
1:B:33:LYS:HE2	3:B:705:MPD:H31	1.83	0.59
1:B:36:LEU:HD21	1:B:55:VAL:CG2	2.32	0.59
1:B:464:ARG:HD2	4:B:1013:HOH:O	2.02	0.59
1:A:483:MET:CE	1:A:606:LEU:HD23	2.31	0.59
1:B:404:PHE:CE2	1:B:604:ILE:HG13	2.37	0.59
1:A:122:LEU:HD23	1:A:222:THR:HA	1.84	0.59
1:A:292:GLN:HG2	1:A:296:MET:HE3	1.85	0.59
1:B:147:HIS:CD2	1:B:445:ARG:HH22	2.20	0.59
1:A:284:HIS:H	1:A:292:GLN:NE2	2.02	0.58
1:B:416:PRO:HB2	1:B:569:ILE:HD13	1.85	0.57
1:B:404:PHE:HB2	1:B:408:LEU:HD13	1.86	0.57
2:B:701:EPE:C10	3:B:702:MPD:H51	2.28	0.57
1:B:222:THR:O	1:B:226:LYS:HG2	2.05	0.56
1:A:442:ALA:HB2	1:A:455:VAL:HG23	1.86	0.56
1:B:263:LEU:O	1:B:267:GLU:HG3	2.05	0.56
1:A:604:ILE:HA	1:A:607:MET:CE	2.36	0.56
1:A:604:ILE:HD13	1:A:607:MET:CE	2.35	0.56
1:B:406:LYS:HB3	1:B:569:ILE:HG21	1.88	0.56
1:A:144:LEU:HD12	1:A:145:PRO:HD2	1.89	0.55
1:A:546:VAL:HG22	1:A:567:TYR:O	2.07	0.55
1:B:406:LYS:HB3	1:B:569:ILE:CG2	2.37	0.55
1:A:546:VAL:CG2	1:A:568:HIS:HB3	2.37	0.54
1:A:144:LEU:HD11	4:A:827:HOH:O	2.07	0.54
1:B:51:THR:OG1	1:B:529:LEU:HD12	2.07	0.54
1:A:555:VAL:HG22	1:A:566:PHE:CZ	2.43	0.54
1:A:373:ASP:O	1:A:377:LEU:HG	2.08	0.54
1:A:459:THR:CG2	1:A:493:MET:HE1	2.38	0.54
1:B:463:VAL:O	1:B:467:GLN:HG3	2.08	0.54
1:B:395:GLN:NE2	4:B:742:HOH:O	2.41	0.53
1:B:401:PHE:CZ	1:B:403:SER:HB2	2.43	0.53
1:B:36:LEU:HD21	1:B:55:VAL:CG1	2.38	0.53
1:B:407:LYS:HD2	1:B:571:ASP:HB2	1.91	0.53
1:A:154:LEU:HD13	1:A:443:MET:HE1	1.90	0.53
1:B:404:PHE:CB	1:B:408:LEU:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ARG:NH2	1:A:382:GLN:NE2	2.57	0.53
1:A:192:ILE:HD11	1:A:203:PHE:CZ	2.44	0.52
1:B:252:ARG:HH21	1:B:270:GLN:NE2	2.02	0.52
1:B:59:GLN:NE2	3:B:705:MPD:H51	2.24	0.51
1:B:302:PRO:HG2	1:B:384:LYS:HG3	1.92	0.51
1:B:214:PRO:HB2	1:B:215:PRO:HD3	1.91	0.51
1:A:372:VAL:HG21	1:A:377:LEU:HD21	1.92	0.51
1:A:402:THR:HG22	1:A:573:ARG:HB3	1.93	0.51
1:B:252:ARG:NH2	1:B:270:GLN:HE22	2.03	0.51
1:B:439:TYR:C	1:B:439:TYR:CD1	2.89	0.50
1:B:36:LEU:O	1:B:39:VAL:HG22	2.10	0.50
1:B:546:VAL:HG12	1:B:546:VAL:O	2.11	0.50
1:A:237:ILE:HD11	1:A:372:VAL:HG11	1.93	0.50
1:B:512:LEU:O	1:B:516:GLU:HG3	2.11	0.50
1:A:51:THR:OG1	1:A:529:LEU:HD12	2.12	0.50
1:A:400:THR:CG2	1:A:573:ARG:HD3	2.42	0.50
1:B:406:LYS:C	1:B:408:LEU:H	2.20	0.50
1:B:555:VAL:HG22	1:B:566:PHE:CZ	2.46	0.50
1:B:112:HIS:HD2	1:B:113:TYR:H	1.58	0.50
1:A:190:THR:O	1:A:205:VAL:HG22	2.11	0.49
1:A:603:MET:O	1:A:607:MET:HG3	2.11	0.49
1:A:122:LEU:CD2	1:A:222:THR:HA	2.42	0.49
1:A:415:HIS:CD2	1:A:417:ASP:H	2.30	0.49
1:B:414:LEU:CD1	1:B:607:MET:SD	3.01	0.49
1:A:585:PRO:HG2	1:A:586:GLU:OE2	2.12	0.49
1:B:327:HIS:NE2	3:B:702:MPD:H52	2.28	0.49
1:B:568:HIS:CE1	1:B:570:ARG:HE	2.28	0.49
1:B:33:LYS:HE3	4:B:1038:HOH:O	2.12	0.49
1:B:265:LEU:HG	1:B:368:LEU:HB3	1.95	0.48
1:B:197:ARG:HA	4:B:930:HOH:O	2.13	0.48
1:B:75:ARG:HA	3:B:706:MPD:HM1	1.95	0.48
1:B:414:LEU:HD13	1:B:487:PHE:CZ	2.49	0.48
1:B:604:ILE:HD13	1:B:607:MET:HE3	1.95	0.48
1:B:117:ARG:HE	1:B:120:THR:HG21	1.79	0.48
1:A:259:ASP:HB3	1:A:262:ASN:ND2	2.29	0.48
1:A:608:ASN:O	1:A:611:HIS:HB3	2.14	0.48
1:A:123:GLU:CD	1:A:123:GLU:N	2.68	0.47
1:B:201:PHE:CE2	1:B:367:GLU:HB2	2.49	0.47
1:B:561:ASN:HA	1:B:584:CYS:SG	2.54	0.47
1:A:604:ILE:HG22	1:A:608:ASN:ND2	2.28	0.47
1:B:182:THR:OG1	1:B:185:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:HG2	1:B:296:MET:HE3	1.97	0.47
1:B:538:ASN:HA	1:B:559:VAL:CG1	2.43	0.47
1:A:600:PHE:O	1:A:604:ILE:HG12	2.14	0.47
1:A:480:GLN:O	1:A:484:LEU:HG	2.14	0.47
1:B:358:LYS:HB3	1:B:358:LYS:HZ2	1.79	0.47
1:A:247:ARG:NH2	1:A:382:GLN:HE22	2.13	0.47
1:A:439:TYR:CD1	1:A:439:TYR:C	2.93	0.47
1:B:29:GLU:O	1:B:33:LYS:HG2	2.15	0.47
1:B:54:ILE:HG23	1:B:523:GLU:HG3	1.95	0.47
1:A:414:LEU:HD12	1:A:607:MET:SD	2.55	0.47
1:A:416:PRO:CB	1:A:569:ILE:HD13	2.41	0.46
1:A:481:GLN:O	1:A:485:GLU:HG3	2.15	0.46
1:B:524:LEU:C	1:B:524:LEU:HD23	2.40	0.46
1:A:107:CYS:HB3	1:A:109:HIS:CE1	2.51	0.46
1:B:513:ILE:O	1:B:517:GLU:HG2	2.15	0.46
1:A:568:HIS:CD2	1:A:575:VAL:HB	2.51	0.46
1:B:442:ALA:HB2	1:B:455:VAL:HG23	1.97	0.46
1:B:604:ILE:HD13	1:B:607:MET:CE	2.45	0.46
1:B:213:THR:HB	1:B:214:PRO:HD2	1.98	0.46
1:B:225:HIS:HE1	4:B:892:HOH:O	1.99	0.46
1:B:415:HIS:CD2	1:B:417:ASP:H	2.34	0.46
1:B:36:LEU:HD21	1:B:55:VAL:CB	2.46	0.45
1:B:109:HIS:HD2	1:B:343:ASP:OD1	1.98	0.45
1:B:407:LYS:HD2	1:B:571:ASP:CB	2.46	0.45
1:B:75:ARG:HG2	3:B:706:MPD:HM1	1.98	0.45
1:B:247:ARG:NH2	1:B:382:GLN:HE22	2.13	0.45
1:B:284:HIS:N	1:B:292:GLN:HE21	2.12	0.45
1:A:400:THR:HG21	1:A:573:ARG:HD3	1.99	0.45
1:A:197:ARG:HG3	1:A:228:CYS:HB3	1.98	0.44
1:A:560:HIS:HE1	1:A:583:SER:OG	1.99	0.44
1:A:604:ILE:HD13	1:A:607:MET:HE1	1.97	0.44
1:B:414:LEU:HD11	1:B:607:MET:SD	2.57	0.44
1:A:554:VAL:HG23	1:A:566:PHE:HD2	1.82	0.44
1:A:593:VAL:O	1:A:596:ILE:HG22	2.17	0.44
1:B:406:LYS:HG3	1:B:407:LYS:N	2.31	0.44
1:B:566:PHE:CE1	3:B:702:MPD:H32	2.53	0.44
1:A:483:MET:HE1	1:A:603:MET:HA	1.99	0.44
1:A:439:TYR:HB2	1:A:539:PHE:CG	2.53	0.44
1:B:406:LYS:HB2	1:B:416:PRO:HG3	2.00	0.44
1:B:230:ASN:O	1:B:231:GLU:HG3	2.17	0.44
1:A:415:HIS:HD2	1:A:417:ASP:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:HIS:HD2	4:A:664:HOH:O	2.01	0.43
1:A:570:ARG:HD2	1:A:573:ARG:HD2	2.00	0.43
1:A:414:LEU:CD1	1:A:607:MET:SD	3.06	0.43
1:A:508:LEU:O	1:A:512:LEU:HG	2.18	0.43
1:B:72:GLU:HG3	4:B:877:HOH:O	2.19	0.43
1:A:609:THR:O	1:A:612:LEU:HD13	2.19	0.43
1:A:106:PRO:HB3	1:A:293:VAL:HG11	2.00	0.43
1:B:294:PHE:CE1	1:B:554:VAL:HG13	2.53	0.43
1:B:408:LEU:HB2	4:B:931:HOH:O	2.18	0.43
1:A:275:VAL:HG23	1:A:309:LYS:HG2	2.01	0.42
1:B:408:LEU:C	1:B:408:LEU:HD23	2.44	0.42
1:A:470:GLN:O	1:A:472:PRO:HD3	2.19	0.42
1:B:293:VAL:O	1:B:297:LEU:HB2	2.19	0.42
1:A:219:ARG:NH2	1:A:220:GLN:HE22	1.95	0.42
1:A:196:CYS:O	1:A:197:ARG:C	2.63	0.42
1:A:459:THR:O	1:A:463:VAL:HG23	2.19	0.42
1:B:49:LYS:O	1:B:53:GLU:HG3	2.20	0.42
1:A:430:ARG:NE	1:A:470:GLN:HE22	2.08	0.42
1:B:49:LYS:HE2	4:B:1033:HOH:O	2.19	0.42
1:A:188:CYS:O	1:A:189:PRO:C	2.63	0.42
1:A:20:LEU:HD11	1:A:155:ASP:HA	2.01	0.42
1:B:284:HIS:N	1:B:292:GLN:NE2	2.53	0.41
1:A:545:LEU:HG	1:A:547:GLY:H	1.85	0.41
1:B:213:THR:HB	1:B:214:PRO:CD	2.50	0.41
1:B:103:PHE:HA	1:B:555:VAL:HG12	2.02	0.41
1:A:136:TRP:HA	1:A:163:PHE:CE2	2.55	0.41
1:A:235:PRO:HG2	4:A:723:HOH:O	2.19	0.41
1:A:140:ARG:HG2	1:A:183:GLU:HG3	2.03	0.41
1:B:49:LYS:HD3	1:B:49:LYS:HA	1.92	0.41
1:B:481:GLN:HE21	1:B:485:GLU:HG3	1.86	0.41
1:A:36:LEU:O	1:A:39:VAL:HG22	2.21	0.41
1:A:106:PRO:HD3	1:A:294:PHE:CE1	2.55	0.41
1:B:400:THR:CG2	1:B:573:ARG:HD3	2.50	0.41
1:A:418:THR:HG23	1:A:490:HIS:HB3	2.03	0.41
1:B:302:PRO:CG	1:B:384:LYS:HG3	2.50	0.41
1:B:570:ARG:HD2	1:B:573:ARG:HD2	2.03	0.41
1:A:40:LYS:HB2	1:A:41:PRO:HD3	2.03	0.40
1:A:611:HIS:O	1:A:612:LEU:OXT	2.39	0.40
1:B:98:GLN:O	1:B:102:ASN:HB2	2.22	0.40
1:B:508:LEU:O	1:B:512:LEU:HG	2.21	0.40
1:A:144:LEU:HD12	1:A:145:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CE2	1:A:367:GLU:HB2	2.57	0.40
1:B:412:GLU:HA	1:B:412:GLU:OE1	2.22	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	587/612 (96%)	570 (97%)	17 (3%)	0	100	100
1	B	598/612 (98%)	582 (97%)	16 (3%)	0	100	100
All	All	1185/1224 (97%)	1152 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	522/541 (96%)	513 (98%)	9 (2%)	53	60
1	B	529/541 (98%)	521 (98%)	8 (2%)	57	64
All	All	1051/1082 (97%)	1034 (98%)	17 (2%)	55	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	69	LYS
1	A	70	LEU
1	A	123	GLU
1	A	248	TRP
1	A	297	LEU
1	A	313	LEU
1	A	330	TYR
1	A	443	MET
1	B	139	LEU
1	B	248	TRP
1	B	265	LEU
1	B	297	LEU
1	B	313	LEU
1	B	330	TYR
1	B	358	LYS
1	B	554	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	59	GLN
1	A	87	ASN
1	A	102	ASN
1	A	109	HIS
1	A	112	HIS
1	A	121	GLN
1	A	131	HIS
1	A	132	ASN
1	A	137	GLN
1	A	220	GLN
1	A	270	GLN
1	A	292	GLN
1	A	378	ASN
1	A	382	GLN
1	A	387	HIS
1	A	415	HIS
1	A	470	GLN
1	A	480	GLN
1	A	490	HIS
1	A	560	HIS
1	A	568	HIS

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Mol	Chain	Res	Type
1	A	594	GLN
1	B	59	GLN
1	B	100	ASN
1	B	102	ASN
1	B	109	HIS
1	B	112	HIS
1	B	121	GLN
1	B	131	HIS
1	B	147	HIS
1	B	151	ASN
1	B	157	ASN
1	B	220	GLN
1	B	225	HIS
1	B	270	GLN
1	B	284	HIS
1	B	292	GLN
1	B	382	GLN
1	B	395	GLN
1	B	415	HIS
1	B	470	GLN
1	B	480	GLN
1	B	481	GLN
1	B	490	HIS
1	B	568	HIS
1	B	594	GLN
1	B	608	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

9 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	EPE	A	613	-	15,15,15	1.34	1 (6%)	19,20,20	0.59	0
3	MPD	B	702	-	7,7,7	0.49	0	9,10,10	0.53	0
3	MPD	B	704	-	7,7,7	0.49	0	9,10,10	0.44	0
3	MPD	B	705	-	7,7,7	0.45	0	9,10,10	0.44	0
3	MPD	B	706	-	7,7,7	0.52	0	9,10,10	0.51	0
3	MPD	B	707	-	7,7,7	0.49	0	9,10,10	0.43	0
3	MPD	B	703	-	7,7,7	0.49	0	9,10,10	0.48	0
2	EPE	B	701	-	15,15,15	1.35	1 (6%)	19,20,20	0.65	0
3	MPD	A	614	-	7,7,7	0.49	0	9,10,10	0.50	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	EPE	A	613	-	-	0/9/19/19	0/1/1/1
3	MPD	B	702	-	-	2/5/5/5	-
3	MPD	B	704	-	-	1/5/5/5	-
3	MPD	B	705	-	-	4/5/5/5	-
3	MPD	B	706	-	-	0/5/5/5	-
3	MPD	B	707	-	-	3/5/5/5	-
3	MPD	B	703	-	-	0/5/5/5	-
2	EPE	B	701	-	-	0/9/19/19	0/1/1/1
3	MPD	A	614	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	613	EPE	C10-S	4.15	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	EPE	C10-S	4.12	1.83	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	MPD	C2-C3-C4-O4
3	B	702	MPD	C2-C3-C4-C5
3	B	705	MPD	C2-C3-C4-O4
3	B	705	MPD	C2-C3-C4-C5
3	B	705	MPD	O2-C2-C3-C4
3	B	707	MPD	O2-C2-C3-C4
3	B	704	MPD	C2-C3-C4-O4
3	B	705	MPD	CM-C2-C3-C4
3	B	707	MPD	C1-C2-C3-C4
3	B	707	MPD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	MPD	4	0
3	B	705	MPD	3	0
3	B	706	MPD	2	0
2	B	701	EPE	2	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, 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	591/612 (96%)	0.55	64 (10%)	11 10	15, 30, 51, 83	0
1	B	600/612 (98%)	-0.13	29 (4%)	35 34	10, 18, 40, 86	0
All	All	1191/1224 (97%)	0.21	93 (7%)	19 18	10, 24, 48, 86	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	408	LEU	7.7
1	A	612	LEU	5.1
1	B	607	MET	5.0
1	B	610	ALA	4.7
1	A	607	MET	4.7
1	B	404	PHE	4.6
1	B	407	LYS	4.5
1	B	409	THR	4.4
1	A	234	GLY	4.3
1	B	601	HIS	4.1
1	A	476	LEU	4.1
1	B	609	THR	4.0
1	A	230	ASN	3.7
1	A	369	VAL	3.6
1	A	123	GLU	3.6
1	A	372	VAL	3.5
1	A	609	THR	3.5
1	A	606	LEU	3.5
1	A	359	VAL	3.5
1	B	406	LYS	3.4
1	B	571	ASP	3.3
1	B	411	GLU	3.2
1	B	517	GLU	3.1
1	A	402	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	223	TYR	3.1
1	A	370	PHE	3.1
1	A	610	ALA	3.0
1	A	258	LEU	2.9
1	B	352	ARG	2.9
1	B	410	LYS	2.8
1	A	233	VAL	2.8
1	A	226	LYS	2.8
1	A	229	SER	2.8
1	B	605	GLN	2.8
1	B	606	LEU	2.8
1	B	76	GLY	2.8
1	B	150	GLY	2.8
1	A	368	LEU	2.8
1	A	53	GLU	2.7
1	A	119	GLY	2.7
1	B	402	THR	2.7
1	A	363	PRO	2.7
1	B	608	ASN	2.7
1	A	227	LYS	2.6
1	B	413	ALA	2.6
1	A	364	LEU	2.6
1	A	362	ILE	2.6
1	A	583	SER	2.6
1	A	608	ASN	2.5
1	B	590	GLU	2.5
1	A	375	LYS	2.5
1	B	405	GLY	2.5
1	A	256	ILE	2.5
1	A	257	SER	2.4
1	A	261	GLU	2.4
1	A	255	LEU	2.4
1	B	395	GLN	2.4
1	A	582	ARG	2.4
1	A	265	LEU	2.4
1	A	260	PRO	2.4
1	B	72	GLU	2.3
1	A	190	THR	2.3
1	A	213	THR	2.3
1	A	254	TYR	2.3
1	A	477	LEU	2.3
1	B	357	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	210	CYS	2.3
1	A	259	ASP	2.3
1	A	187	HIS	2.2
1	A	207	HIS	2.2
1	A	358	LYS	2.2
1	A	376	ILE	2.2
1	A	228	CYS	2.2
1	A	221	LEU	2.2
1	A	117	ARG	2.2
1	A	604	ILE	2.2
1	A	200	ALA	2.2
1	A	573	ARG	2.2
1	A	222	THR	2.2
1	A	202	VAL	2.1
1	A	231	GLU	2.1
1	A	601	HIS	2.1
1	A	121	GLN	2.1
1	A	611	HIS	2.1
1	B	12	ARG	2.1
1	A	208	GLU	2.1
1	A	395	GLN	2.1
1	B	209	GLY	2.1
1	A	118	GLU	2.0
1	A	232	PRO	2.0
1	B	230	ASN	2.0
1	A	211	LEU	2.0
1	A	12	ARG	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 oligosaccharides 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, 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	MPD	B	706	8/8	0.80	0.21	63,64,65,65	0
3	MPD	B	704	8/8	0.81	0.24	75,75,75,75	0
3	MPD	B	705	8/8	0.82	0.24	66,67,67,67	0
3	MPD	A	614	8/8	0.82	0.13	31,33,36,36	0
3	MPD	B	707	8/8	0.82	0.19	37,40,40,42	0
3	MPD	B	702	8/8	0.85	0.12	14,20,23,23	0
3	MPD	B	703	8/8	0.88	0.15	39,40,42,44	0
2	EPE	A	613	15/15	0.95	0.10	20,26,34,36	0
2	EPE	B	701	15/15	0.97	0.09	15,23,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.