



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:19 AM UTC

PDB ID : 6M5O / pdb_00006m5o
Title : Co-crystal structure of human serine hydroxymethyltransferase 2 in complex with Pyridoxal 5'-phosphate (PLP) and glycodeoxycholic acid
Authors : Ota, T.; Senoo, A.; Ito, S.; Ueno, G.; Nagatoishi, S.; Tsumoto, K.; Sando, S.
Deposited on : 2020-03-11
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

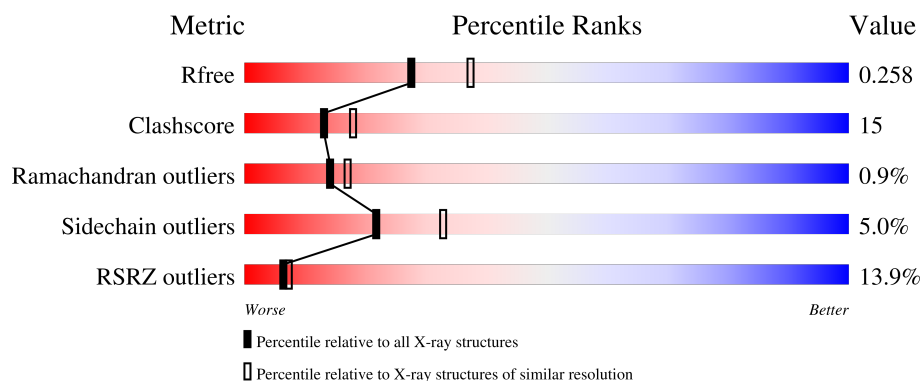
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	507	
1	B	507	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7878 atoms, of which 84 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	P	S	0	0	0
			3622	2281	649	675	1	16			
1	B	462	Total	C	N	O	P	S	0	0	0
			3618	2278	648	675	1	16			

There are 38 discrepancies between the modelled and reference sequences:

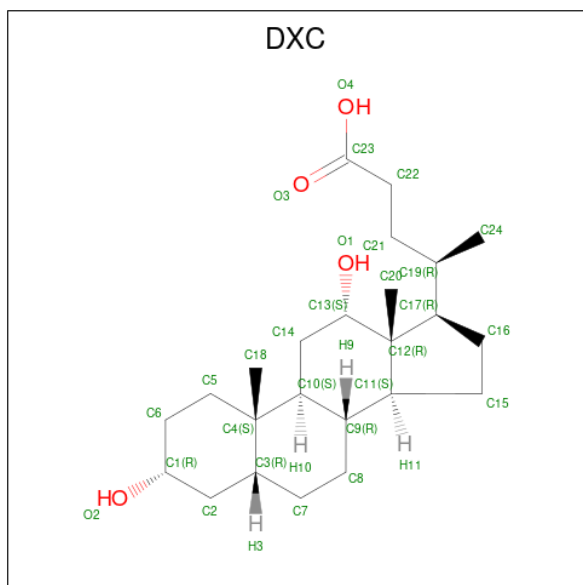
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P34897
A	-1	GLY	-	expression tag	UNP P34897
A	0	SER	-	expression tag	UNP P34897
A	1	SER	-	expression tag	UNP P34897
A	2	HIS	-	expression tag	UNP P34897
A	3	HIS	-	expression tag	UNP P34897
A	4	HIS	-	expression tag	UNP P34897
A	5	HIS	-	expression tag	UNP P34897
A	6	HIS	-	expression tag	UNP P34897
A	7	HIS	-	expression tag	UNP P34897
A	8	SER	-	expression tag	UNP P34897
A	9	SER	-	expression tag	UNP P34897
A	10	GLY	-	expression tag	UNP P34897
A	11	LEU	-	expression tag	UNP P34897
A	12	VAL	-	expression tag	UNP P34897
A	13	PRO	-	expression tag	UNP P34897
A	14	ARG	-	expression tag	UNP P34897
A	15	GLY	-	expression tag	UNP P34897
A	16	SER	-	expression tag	UNP P34897
B	-2	MET	-	expression tag	UNP P34897
B	-1	GLY	-	expression tag	UNP P34897
B	0	SER	-	expression tag	UNP P34897
B	1	SER	-	expression tag	UNP P34897
B	2	HIS	-	expression tag	UNP P34897
B	3	HIS	-	expression tag	UNP P34897

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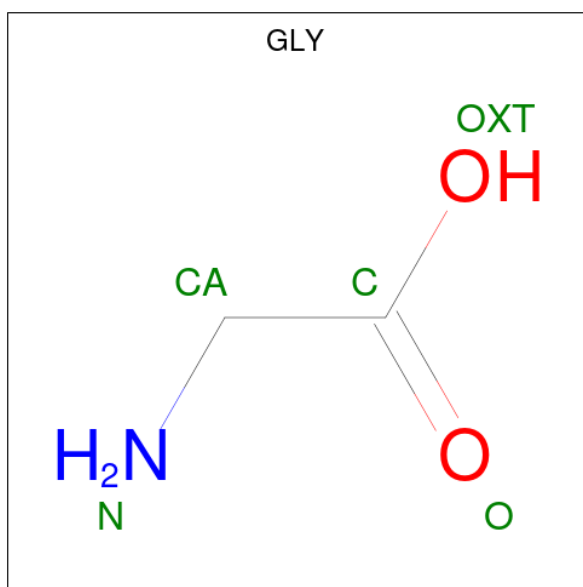
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP P34897
B	5	HIS	-	expression tag	UNP P34897
B	6	HIS	-	expression tag	UNP P34897
B	7	HIS	-	expression tag	UNP P34897
B	8	SER	-	expression tag	UNP P34897
B	9	SER	-	expression tag	UNP P34897
B	10	GLY	-	expression tag	UNP P34897
B	11	LEU	-	expression tag	UNP P34897
B	12	VAL	-	expression tag	UNP P34897
B	13	PRO	-	expression tag	UNP P34897
B	14	ARG	-	expression tag	UNP P34897
B	15	GLY	-	expression tag	UNP P34897
B	16	SER	-	expression tag	UNP P34897

- Molecule 2 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (CCD ID: DXC) (formula: $C_{24}H_{40}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			66	24	39	3		
2	A	1	Total	C	H	O	0	0
			66	24	39	3		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



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

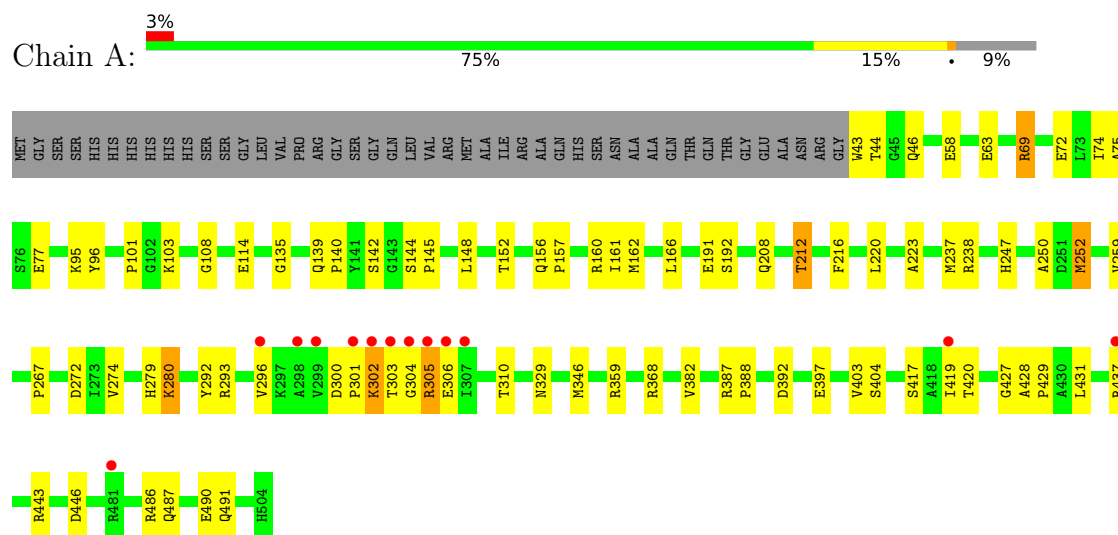
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		
4	B	170	Total	O	0	0
			170	170		

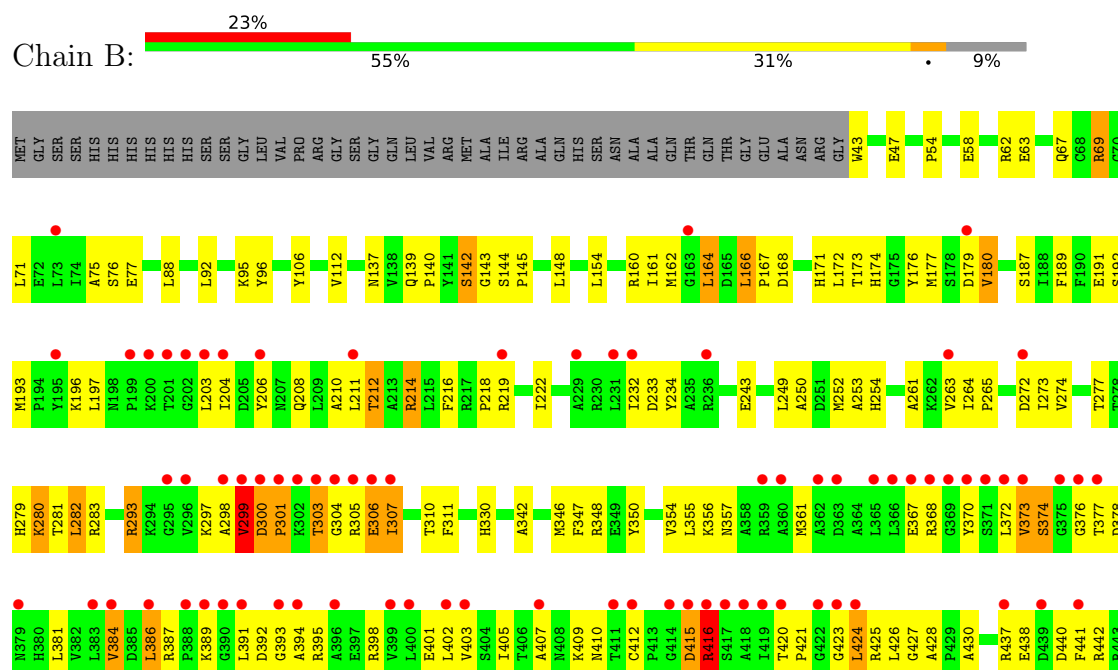
3 Residue-property plots

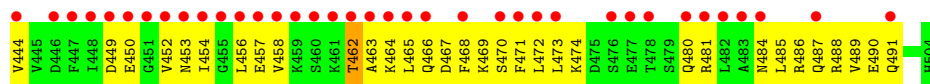
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.84Å 159.84Å 211.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.36 – 2.30 49.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.36-2.30) 100.0 (49.36-2.30)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11	Depositor
R, R_{free}	0.201 , 0.256 0.203 , 0.258	Depositor DCC
R_{free} test set	3516 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7878	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/3670	0.56	0/4964
1	B	0.29	0/3666	0.54	0/4960
All	All	0.33	0/7336	0.55	0/9924

There are no bond length outliers.

There are no bond angle outliers.

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	3622	0	3609	67	0
1	B	3618	0	3598	157	0
2	A	54	78	78	3	0
3	A	5	3	2	0	0
3	B	5	3	2	0	0
4	A	320	0	0	6	0
4	B	170	0	0	9	0
All	All	7794	84	7289	217	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 15.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HH22	1:B:346:MET:HE1	1.24	1.02
1:B:372:LEU:HD12	1:B:376:GLY:HA2	1.55	0.88
1:B:470:SER:O	1:B:474:LYS:HD3	1.78	0.84
1:B:370:TYR:OH	1:B:452:VAL:HG11	1.78	0.83
1:B:368:ARG:HD3	1:B:449:ASP:OD2	1.79	0.82
1:A:223:ALA:HB2	1:A:237:MET:HE2	1.62	0.81
1:B:166:LEU:HD23	1:B:176:TYR:HB2	1.64	0.80
1:A:162:MET:HE1	1:A:212:THR:CG2	2.11	0.79
1:A:252:MET:HE1	1:A:259:VAL:HG11	1.65	0.79
1:A:212:THR:HG21	4:A:795:HOH:O	1.84	0.77
1:B:373:VAL:O	1:B:374:SER:HB3	1.85	0.75
1:B:283:ARG:NH2	1:B:346:MET:HE1	2.00	0.74
1:B:143:GLY:HA3	1:B:280:LLP:H5'2	1.69	0.74
1:B:485:LEU:O	1:B:489:VAL:HG23	1.88	0.73
1:B:63:GLU:O	1:B:67:GLN:HG3	1.89	0.72
1:B:384:VAL:HG23	1:B:386:LEU:HD13	1.71	0.72
1:B:458:VAL:HG13	1:B:471:PHE:CD2	2.24	0.72
1:B:357:ASN:HB3	1:B:441:PHE:CE1	2.25	0.72
1:B:361:MET:HE2	1:B:426:LEU:HD13	1.72	0.70
1:B:214:ARG:NH2	1:B:243:GLU:OE2	2.24	0.70
1:B:466:GLN:HG2	4:B:715:HOH:O	1.91	0.70
1:A:300:ASP:HB3	1:A:303:THR:O	1.93	0.69
1:B:272:ASP:HA	1:B:293:ARG:HG3	1.75	0.68
1:A:420:THR:O	1:A:420:THR:HG22	1.91	0.68
1:B:206:TYR:CE2	1:B:233:ASP:HB3	2.29	0.67
1:B:454:ILE:O	1:B:458:VAL:HG23	1.95	0.67
1:B:389:LYS:O	1:B:456:LEU:HD21	1.95	0.67
1:A:252:MET:HE2	1:A:259:VAL:HG21	1.78	0.66
1:B:162:MET:HE1	1:B:212:THR:CG2	2.25	0.66
1:B:300:ASP:H	1:B:301:PRO:HD3	1.60	0.66
1:B:299:VAL:HG22	1:B:299:VAL:O	1.94	0.66
1:B:415:ASP:O	1:B:416:ARG:HD2	1.96	0.66
1:A:392:ASP:CB	1:A:420:THR:HG23	2.27	0.64
1:A:148:LEU:O	1:A:152:THR:HG23	1.98	0.64
1:A:305:ARG:O	1:A:306:GLU:HB2	1.96	0.64
1:B:299:VAL:HG21	1:B:304:GLY:HA2	1.79	0.64
1:B:95:LYS:HG2	1:B:112:VAL:HG11	1.80	0.63
1:B:372:LEU:CD1	1:B:376:GLY:HA2	2.28	0.63
1:B:299:VAL:CG2	1:B:304:GLY:HA2	2.29	0.63
1:A:166:LEU:HD23	2:A:601:DXC:H183	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLY:O	1:A:306:GLU:N	2.32	0.62
1:B:210:ALA:O	1:B:214:ARG:HG2	1.99	0.62
1:B:392:ASP:OD1	1:B:395:ARG:HD2	2.00	0.62
1:B:484:ASN:OD1	1:B:488:ARG:NH1	2.33	0.61
1:A:252:MET:CE	1:A:259:VAL:HG21	2.29	0.61
1:B:470:SER:HB2	1:B:474:LYS:HZ3	1.65	0.61
1:A:162:MET:HE1	1:A:212:THR:HG22	1.81	0.60
1:A:95:LYS:HE2	1:A:108:GLY:O	2.02	0.60
1:B:398:ARG:HG3	1:B:472:LEU:HD12	1.83	0.60
1:B:387:ARG:HA	4:B:723:HOH:O	2.02	0.59
1:B:464:LYS:HB2	4:B:703:HOH:O	2.02	0.59
1:B:438:GLU:OE1	1:B:438:GLU:N	2.28	0.59
1:B:280:LLP:NZ	1:B:280:LLP:O3	2.31	0.59
1:B:457:GLU:OE1	1:B:481:ARG:NH1	2.32	0.59
1:B:154:LEU:HD11	1:B:273:ILE:HD12	1.84	0.59
1:B:76:SER:O	1:B:280:LLP:HG3	2.03	0.59
1:B:470:SER:HB2	1:B:474:LYS:NZ	2.18	0.59
1:A:114:GLU:CD	1:B:62:ARG:HH22	2.12	0.58
1:B:373:VAL:O	1:B:374:SER:CB	2.52	0.58
1:A:346:MET:HE2	1:B:43:TRP:CD1	2.37	0.58
1:A:69:ARG:HD2	1:A:490:GLU:OE2	2.04	0.58
1:A:301:PRO:O	1:A:302:LYS:HB2	2.02	0.58
1:B:168:ASP:OD2	1:B:197:LEU:HB2	2.05	0.57
1:A:487:GLN:O	1:A:491:GLN:HG3	2.04	0.57
1:B:272:ASP:HB3	1:B:311:PHE:CE2	2.40	0.57
1:B:350:TYR:O	1:B:354:VAL:HG23	2.04	0.57
1:B:164:LEU:HD11	1:B:168:ASP:O	2.05	0.57
1:A:238:ARG:O	1:A:238:ARG:HD3	2.05	0.57
1:B:162:MET:HE1	1:B:212:THR:HG23	1.86	0.57
1:B:162:MET:HG3	1:B:218:PRO:HB3	1.87	0.57
1:A:368:ARG:NH1	1:A:446:ASP:OD1	2.36	0.56
1:B:412:CYS:N	1:B:415:ASP:OD2	2.32	0.56
1:B:458:VAL:O	1:B:462:THR:OG1	2.23	0.56
1:B:137:ASN:OD1	1:B:140:PRO:HD3	2.06	0.56
1:B:300:ASP:H	1:B:301:PRO:CD	2.18	0.56
1:B:154:LEU:HD11	1:B:273:ILE:CD1	2.36	0.56
1:B:298:ALA:O	1:B:307:ILE:HG13	2.06	0.56
1:B:357:ASN:HB3	1:B:441:PHE:CD1	2.42	0.55
1:B:438:GLU:O	1:B:442:ARG:HG3	2.07	0.55
1:B:300:ASP:N	1:B:301:PRO:CD	2.69	0.54
1:A:208:GLN:O	1:A:212:THR:HB	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:PRO:HD2	4:B:753:HOH:O	2.06	0.54
1:B:387:ARG:NH1	1:B:415:ASP:H	2.05	0.54
1:A:152:THR:HG22	1:B:189:PHE:HZ	1.72	0.54
1:A:403:VAL:HA	1:A:486:ARG:HB2	1.90	0.54
1:B:177:MET:HE2	1:B:187:SER:HB3	1.88	0.54
1:A:252:MET:HE3	1:A:267:PRO:CG	2.37	0.54
1:B:393:GLY:HA3	1:B:423:GLY:O	2.08	0.54
1:A:417:SER:OG	1:A:419:ILE:HG12	2.08	0.53
1:B:166:LEU:CD2	1:B:176:TYR:HB2	2.38	0.53
1:B:263:VAL:CG1	1:B:355:LEU:CD1	2.86	0.52
1:B:395:ARG:HB3	1:B:468:PHE:CZ	2.44	0.52
1:B:450:GLU:OE1	1:B:488:ARG:NH2	2.43	0.52
1:A:74:ILE:HB	1:A:77:GLU:HG3	1.91	0.52
1:B:465:LEU:O	1:B:469:LYS:HG3	2.09	0.52
1:B:277:THR:HB	1:B:279:HIS:CE1	2.45	0.52
1:A:280:LLP:NZ	1:A:280:LLP:O3	2.31	0.51
1:A:238:ARG:HH22	1:A:272:ASP:CG	2.18	0.51
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.93	0.51
1:B:139:GLN:N	1:B:140:PRO:CD	2.74	0.51
1:B:485:LEU:O	1:B:485:LEU:HD12	2.09	0.51
1:A:392:ASP:CG	1:A:420:THR:HG23	2.36	0.50
1:A:139:GLN:N	1:A:140:PRO:CD	2.74	0.50
1:A:238:ARG:HD3	1:A:238:ARG:C	2.35	0.50
1:B:463:ALA:HB3	1:B:467:ASP:OD1	2.11	0.50
1:B:232:ILE:HB	1:B:234:TYR:CZ	2.47	0.50
1:A:160:ARG:HA	1:A:191:GLU:O	2.11	0.50
1:B:420:THR:HG22	1:B:420:THR:O	2.11	0.50
1:A:387:ARG:HB2	1:A:388:PRO:HD3	1.94	0.50
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.48	0.49
1:B:441:PHE:O	1:B:444:VAL:HB	2.12	0.49
1:B:69:ARG:HD2	1:B:490:GLU:OE2	2.13	0.49
2:A:601:DXC:H13	2:A:601:DXC:H242	1.94	0.49
1:B:398:ARG:HD2	1:B:398:ARG:O	2.13	0.49
1:B:401:GLU:HA	1:B:405:ILE:O	2.13	0.49
1:A:252:MET:HE1	1:A:259:VAL:CG1	2.41	0.48
1:B:254:HIS:O	1:B:281:THR:HG23	2.13	0.48
1:B:264:ILE:HB	1:B:265:PRO:CD	2.43	0.48
1:B:250:ALA:O	1:B:274:VAL:HA	2.13	0.48
1:B:449:ASP:HA	1:B:452:VAL:HG12	1.94	0.48
1:A:43:TRP:CD2	1:B:346:MET:HE3	2.49	0.47
1:B:166:LEU:HD21	1:B:172:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:THR:OG1	1:B:378:ASP:N	2.47	0.47
1:A:166:LEU:HD23	2:A:601:DXC:C18	2.44	0.47
1:A:403:VAL:O	1:A:404:SER:HB2	2.14	0.47
1:A:428:ALA:N	1:A:429:PRO:CD	2.76	0.47
1:B:437:ARG:HB3	4:B:750:HOH:O	2.14	0.47
1:B:384:VAL:CG2	1:B:386:LEU:HD13	2.43	0.47
1:B:394:ALA:HB2	1:B:421:PRO:HD2	1.97	0.47
1:B:403:VAL:HA	1:B:486:ARG:HG3	1.97	0.47
1:B:249:LEU:HD13	1:B:273:ILE:HG22	1.97	0.46
1:A:237:MET:HE3	1:A:237:MET:HB3	1.88	0.46
1:B:263:VAL:HG12	1:B:355:LEU:HD11	1.97	0.46
1:B:263:VAL:HG11	1:B:355:LEU:HG	1.98	0.46
1:B:402:LEU:HD11	1:B:473:LEU:HD21	1.96	0.46
1:B:166:LEU:CB	1:B:167:PRO:HD3	2.45	0.46
1:B:409:LYS:HA	1:B:424:LEU:HD12	1.97	0.46
1:B:307:ILE:HG13	1:B:307:ILE:H	1.49	0.46
1:B:179:ASP:O	1:B:180:VAL:HG13	2.16	0.45
1:B:480:GLN:HA	4:B:735:HOH:O	2.15	0.45
1:A:162:MET:HE1	1:A:212:THR:HG23	1.95	0.45
1:A:250:ALA:O	1:A:274:VAL:HA	2.16	0.45
1:B:487:GLN:O	1:B:491:GLN:HB2	2.16	0.45
1:B:279:HIS:O	1:B:280:LLP:HB3	2.15	0.45
1:A:72:GLU:HB2	4:A:891:HOH:O	2.17	0.45
1:B:71:LEU:HD12	1:B:489:VAL:HG13	1.98	0.45
1:B:303:THR:HB	1:B:304:GLY:H	1.45	0.45
1:A:44:THR:OG1	1:A:46:GLN:HB2	2.17	0.45
1:A:443:ARG:NH1	4:A:711:HOH:O	2.49	0.45
1:B:452:VAL:HG13	1:B:453:ASN:N	2.32	0.45
1:B:470:SER:C	1:B:474:LYS:HD3	2.41	0.45
1:B:249:LEU:CD1	1:B:273:ILE:HG22	2.48	0.44
1:B:299:VAL:O	1:B:299:VAL:CG2	2.63	0.44
1:B:252:MET:O	1:B:253:ALA:C	2.60	0.44
1:A:220:LEU:HD12	1:A:247:HIS:HB2	2.00	0.44
1:B:171:HIS:CE1	1:B:173:THR:HG23	2.53	0.44
1:B:342:ALA:HA	1:B:347:PHE:CG	2.52	0.44
1:A:144:SER:HB2	1:A:145:PRO:HD3	1.99	0.44
1:B:392:ASP:CG	1:B:420:THR:HG23	2.42	0.44
1:A:135:GLY:HA3	1:A:292:TYR:CE1	2.53	0.44
1:A:156:GLN:O	1:A:157:PRO:C	2.60	0.44
1:A:397:GLU:OE2	1:B:106:TYR:HA	2.18	0.44
1:B:144:SER:HB2	1:B:145:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:CG2	1:B:384:VAL:O	2.66	0.44
1:B:441:PHE:O	1:B:444:VAL:N	2.50	0.44
1:A:43:TRP:CE3	1:B:346:MET:HE3	2.53	0.44
1:A:306:GLU:HA	1:A:306:GLU:OE1	2.17	0.44
1:A:310:THR:HG22	1:A:310:THR:O	2.18	0.44
1:B:381:LEU:C	1:B:381:LEU:HD12	2.42	0.43
1:A:359:ARG:NH1	4:A:716:HOH:O	2.51	0.43
1:B:250:ALA:HB3	1:B:274:VAL:HG22	2.01	0.43
1:B:261:ALA:HB1	1:B:348:ARG:HA	2.00	0.43
1:B:387:ARG:HH12	1:B:415:ASP:H	1.65	0.43
1:B:222:ILE:HG12	1:B:249:LEU:HD23	2.01	0.43
1:B:305:ARG:O	1:B:306:GLU:C	2.61	0.43
1:B:279:HIS:HB2	4:B:759:HOH:O	2.17	0.43
1:B:391:LEU:HD23	1:B:452:VAL:HG23	2.00	0.43
1:B:370:TYR:CE1	1:B:389:LYS:HD3	2.54	0.43
1:B:384:VAL:HG23	1:B:384:VAL:O	2.19	0.43
1:A:160:ARG:HD3	1:A:216:PHE:CE1	2.54	0.43
1:B:437:ARG:N	1:B:440:ASP:OD2	2.49	0.43
1:A:428:ALA:N	1:A:429:PRO:HD3	2.33	0.42
1:B:468:PHE:O	1:B:472:LEU:HG	2.19	0.42
1:A:95:LYS:HD2	1:B:77:GLU:OE2	2.19	0.42
1:A:139:GLN:N	1:A:140:PRO:HD3	2.35	0.42
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.82	0.42
1:A:161:ILE:O	1:A:192:SER:HA	2.19	0.42
1:B:452:VAL:O	1:B:456:LEU:N	2.37	0.42
1:B:208:GLN:O	1:B:211:LEU:N	2.52	0.42
1:B:424:LEU:HD12	1:B:424:LEU:HA	1.81	0.42
1:B:161:ILE:O	1:B:192:SER:HA	2.20	0.42
1:B:415:ASP:O	1:B:416:ARG:CD	2.65	0.42
1:B:470:SER:O	1:B:474:LYS:HB2	2.19	0.42
1:B:160:ARG:HA	1:B:191:GLU:O	2.19	0.42
1:B:204:ILE:O	1:B:206:TYR:CD1	2.73	0.42
1:B:381:LEU:HD22	1:B:425:ARG:HD2	2.00	0.42
1:B:407:ALA:HB1	1:B:425:ARG:O	2.20	0.42
1:B:47:GLU:H	1:B:47:GLU:CD	2.28	0.42
1:B:450:GLU:O	1:B:454:ILE:HD12	2.19	0.42
1:A:63:GLU:HG2	1:B:92:LEU:HD23	2.02	0.41
1:B:88:LEU:O	1:B:330:HIS:HB2	2.19	0.41
1:B:208:GLN:HG2	4:B:843:HOH:O	2.20	0.41
1:B:470:SER:O	1:B:474:LYS:CD	2.59	0.41
1:A:101:PRO:C	1:A:103:LYS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB2	4:A:740:HOH:O	2.18	0.41
1:B:160:ARG:HB2	1:B:218:PRO:HA	2.01	0.41
1:B:162:MET:SD	1:B:218:PRO:HG3	2.60	0.41
1:B:142:SER:C	1:B:145:PRO:HD2	2.46	0.41
1:B:282:LEU:HA	1:B:282:LEU:HD23	1.69	0.41
1:A:279:HIS:HB2	4:A:775:HOH:O	2.21	0.41
1:B:428:ALA:O	1:B:430:ALA:N	2.54	0.41
1:B:193:MET:HE1	1:B:216:PHE:HB2	2.03	0.41
1:B:469:LYS:HE2	4:B:845:HOH:O	2.21	0.41
1:B:297:LYS:O	1:B:298:ALA:HB2	2.21	0.40
1:B:410:ASN:O	1:B:421:PRO:HB2	2.21	0.40
1:A:252:MET:HE3	1:A:267:PRO:HG2	2.03	0.40
1:B:75:ALA:HA	1:B:427:GLY:HA3	2.04	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	459/507 (90%)	441 (96%)	16 (4%)	2 (0%)	30	38
1	B	459/507 (90%)	421 (92%)	32 (7%)	6 (1%)	9	10
All	All	918/1014 (90%)	862 (94%)	48 (5%)	8 (1%)	14	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	B	301	PRO
1	B	416	ARG
1	B	299	VAL
1	A	305	ARG

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Mol	Chain	Res	Type
1	B	374	SER
1	B	180	VAL
1	B	306	GLU

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	380/414 (92%)	370 (97%)	10 (3%)	40	59
1	B	379/414 (92%)	351 (93%)	28 (7%)	13	17
All	All	759/828 (92%)	721 (95%)	38 (5%)	22	33

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	69	ARG
1	A	96	TYR
1	A	142	SER
1	A	212	THR
1	A	252	MET
1	A	293	ARG
1	A	296	VAL
1	A	382	VAL
1	A	437	ARG
1	B	58	GLU
1	B	69	ARG
1	B	96	TYR
1	B	142	SER
1	B	148	LEU
1	B	164	LEU
1	B	166	LEU
1	B	196	LYS
1	B	203	LEU
1	B	212	THR

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Mol	Chain	Res	Type
1	B	214	ARG
1	B	219	ARG
1	B	282	LEU
1	B	293	ARG
1	B	299	VAL
1	B	300	ASP
1	B	303	THR
1	B	307	ILE
1	B	310	THR
1	B	356	LYS
1	B	367	GLU
1	B	373	VAL
1	B	384	VAL
1	B	386	LEU
1	B	415	ASP
1	B	416	ARG
1	B	424	LEU
1	B	462	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	A	466	GLN
1	A	487	GLN
1	A	491	GLN
1	B	61	GLN
1	B	156	GLN
1	B	329	ASN
1	B	353	GLN
1	B	357	ASN
1	B	435	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	LLP	B	280	1	23,24,25	2.42	6 (26%)	25,32,34	1.70	5 (20%)
1	LLP	A	280	1	23,24,25	2.36	6 (26%)	25,32,34	1.84	7 (28%)

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
1	LLP	B	280	1	-	9/16/17/19	0/1/1/1
1	LLP	A	280	1	-	6/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	LLP	C4-C4'	7.26	1.62	1.46
1	A	280	LLP	C4-C4'	6.80	1.61	1.46
1	B	280	LLP	C4'-NZ	5.22	1.44	1.27
1	A	280	LLP	C4'-NZ	4.78	1.43	1.27
1	A	280	LLP	C2'-C2	3.75	1.56	1.50
1	B	280	LLP	C2'-C2	3.38	1.55	1.50
1	A	280	LLP	C6-N1	3.06	1.40	1.34
1	B	280	LLP	C6-N1	2.94	1.40	1.34
1	B	280	LLP	C4-C5	-2.93	1.37	1.42
1	B	280	LLP	C5'-C5	2.32	1.57	1.50
1	A	280	LLP	C4-C5	-2.28	1.38	1.42
1	A	280	LLP	P-OP2	-2.05	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	LLP	C4-C4'-NZ	-4.62	102.71	124.04
1	A	280	LLP	OP4-C5'-C5	4.51	117.82	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LLP	C4-C4'-NZ	-4.26	104.39	124.04
1	A	280	LLP	C5'-C5-C6	-3.29	114.00	119.36
1	B	280	LLP	OP4-C5'-C5	3.21	115.38	109.36
1	B	280	LLP	C3-C4-C4'	-2.94	115.09	120.40
1	B	280	LLP	C5-C4-C4'	2.64	125.54	121.47
1	A	280	LLP	C3-C4-C4'	-2.42	116.04	120.40
1	B	280	LLP	C5'-C5-C6	-2.41	115.43	119.36
1	A	280	LLP	C5-C6-N1	-2.32	120.06	123.83
1	A	280	LLP	OP3-P-OP4	2.27	112.60	106.67
1	A	280	LLP	C5-C4-C4'	2.22	124.90	121.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	LLP	O-C-CA-CB
1	B	280	LLP	C4-C5-C5'-OP4
1	B	280	LLP	C6-C5-C5'-OP4
1	B	280	LLP	C5'-OP4-P-OP1
1	B	280	LLP	C5'-OP4-P-OP2
1	B	280	LLP	C5'-OP4-P-OP3
1	B	280	LLP	O-C-CA-CB
1	A	280	LLP	C4-C4'-NZ-CE
1	B	280	LLP	C4-C4'-NZ-CE
1	A	280	LLP	C5'-OP4-P-OP1
1	B	280	LLP	CD-CE-NZ-C4'
1	B	280	LLP	C3-C4-C4'-NZ
1	A	280	LLP	C5'-OP4-P-OP2
1	A	280	LLP	C3-C4-C4'-NZ
1	A	280	LLP	CD-CE-NZ-C4'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	280	LLP	4	0
1	A	280	LLP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	$\# Z > 2$
3	GLY	B	601	2	4,4,4	1.03	0	3,4,4	1.10	0
2	DXC	A	601	3	29,30,31	0.33	0	47,47,49	0.63	0
3	GLY	A	603	2	4,4,4	1.10	0	3,4,4	1.02	0
2	DXC	A	602	3	29,30,31	0.43	0	47,47,49	0.64	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
3	GLY	B	601	2	-	0/2/2/2	-
2	DXC	A	601	3	-	0/8/70/71	0/4/4/4
3	GLY	A	603	2	-	0/2/2/2	-
2	DXC	A	602	3	-	0/8/70/71	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DXC	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, 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	461/507 (90%)	-0.36	13 (2%) 55 57	16, 26, 56, 140	0
1	B	461/507 (90%)	1.01	115 (24%) 2 2	24, 51, 92, 185	0
All	All	922/1014 (90%)	0.32	128 (13%) 6 7	16, 37, 82, 185	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	GLY	7.5
1	B	418	ALA	6.2
1	A	299	VAL	5.9
1	B	303	THR	5.9
1	B	301	PRO	5.0
1	B	299	VAL	4.8
1	B	307	ILE	4.4
1	B	471	PHE	4.4
1	A	304	GLY	4.4
1	A	301	PRO	4.3
1	B	304	GLY	4.3
1	B	399	VAL	4.2
1	B	460	SER	4.2
1	B	298	ALA	4.2
1	B	391	LEU	4.2
1	B	367	GLU	4.2
1	B	366	LEU	4.1
1	B	200	LYS	4.1
1	B	383	LEU	3.9
1	A	298	ALA	3.9
1	B	441	PHE	3.8
1	B	414	GLY	3.6
1	B	384	VAL	3.6
1	B	462	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	302	LYS	3.6
1	A	306	GLU	3.6
1	B	419	ILE	3.6
1	B	422	GLY	3.5
1	B	455	GLY	3.5
1	B	468	PHE	3.5
1	B	393	GLY	3.4
1	B	449	ASP	3.4
1	B	372	LEU	3.3
1	B	417	SER	3.3
1	B	482	LEU	3.3
1	B	478	THR	3.3
1	B	369	GLY	3.3
1	B	447	PHE	3.3
1	A	481	ARG	3.3
1	B	296	VAL	3.3
1	B	472	LEU	3.2
1	B	476	SER	3.2
1	B	300	ASP	3.2
1	B	459	LYS	3.2
1	B	465	LEU	3.1
1	A	303	THR	3.0
1	B	452	VAL	3.0
1	A	302	LYS	3.0
1	B	389	LYS	3.0
1	B	416	ARG	3.0
1	B	477	GLU	3.0
1	B	473	LEU	3.0
1	B	179	ASP	2.9
1	B	229	ALA	2.9
1	B	396	ALA	2.9
1	B	211	LEU	2.9
1	B	362	ALA	2.9
1	B	219	ARG	2.8
1	B	206	TYR	2.8
1	B	480	GLN	2.8
1	B	481	ARG	2.8
1	B	484	ASN	2.8
1	B	461	LYS	2.8
1	B	359	ARG	2.8
1	A	296	VAL	2.8
1	B	390	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	232	ILE	2.7
1	B	453	ASN	2.7
1	B	463	ALA	2.7
1	B	371	SER	2.7
1	B	411	THR	2.6
1	B	204	ILE	2.6
1	B	375	GLY	2.6
1	B	400	LEU	2.6
1	A	419	ILE	2.6
1	B	394	ALA	2.6
1	B	464	LYS	2.6
1	B	305	ARG	2.6
1	B	306	GLU	2.5
1	B	424	LEU	2.5
1	B	448	ILE	2.5
1	B	456	LEU	2.5
1	B	388	PRO	2.5
1	A	437	ARG	2.4
1	B	420	THR	2.4
1	B	457	GLU	2.4
1	B	195	TYR	2.4
1	B	370	TYR	2.4
1	B	373	VAL	2.4
1	B	386	LEU	2.4
1	B	415	ASP	2.4
1	B	470	SER	2.4
1	B	365	LEU	2.4
1	B	458	VAL	2.4
1	B	368	ARG	2.4
1	B	450	GLU	2.4
1	B	407	ALA	2.3
1	B	403	VAL	2.3
1	B	439	ASP	2.3
1	B	163	GLY	2.3
1	B	202	GLY	2.3
1	B	444	VAL	2.3
1	B	360	ALA	2.3
1	B	466	GLN	2.3
1	B	491	GLN	2.3
1	B	454	ILE	2.3
1	B	203	LEU	2.2
1	B	412	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	201	THR	2.2
1	B	263	VAL	2.2
1	A	305	ARG	2.2
1	B	446	ASP	2.2
1	B	73	LEU	2.2
1	B	379	ASN	2.2
1	B	402	LEU	2.1
1	B	272	ASP	2.1
1	B	363	ASP	2.1
1	B	483	ALA	2.1
1	B	231	LEU	2.1
1	B	295	GLY	2.1
1	B	451	GLY	2.1
1	B	236	ARG	2.1
1	A	307	ILE	2.1
1	B	437	ARG	2.1
1	B	377	THR	2.0
1	B	423	GLY	2.0
1	B	487	GLN	2.0
1	B	199	PRO	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
1	LLP	B	280	24/25	0.96	0.09	31,43,50,54	0
1	LLP	A	280	24/25	0.98	0.05	15,20,26,31	0

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
2	DXC	A	602	27/28	0.86	0.13	24,48,66,67	0
3	GLY	B	601	5/5	0.91	0.09	24,30,32,39	0
2	DXC	A	601	27/28	0.95	0.08	17,29,46,75	66
3	GLY	A	603	5/5	0.99	0.03	14,17,24,24	8

6.5 Other polymers [i](#)

There are no such residues in this entry.