



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:56 AM GMT

PDB ID : 2JEY
Title : MUS MUSCULUS ACETYLCHOLINESTERASE IN COMPLEX WITH HLO-7
Authors : Ekstrom, F.; Astot, C.; Pang, Y.P.
Deposited on : 2007-01-25
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

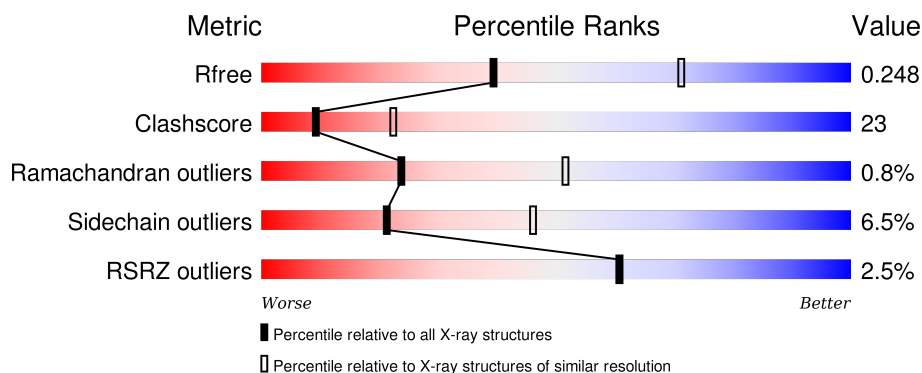
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	548	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>••</div> </div> </div>
1	B	548	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>39%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HLO	B	1545	-	-	-	X
3	P6G	B	1546	-	-	-	X

2 Entry composition [i](#)

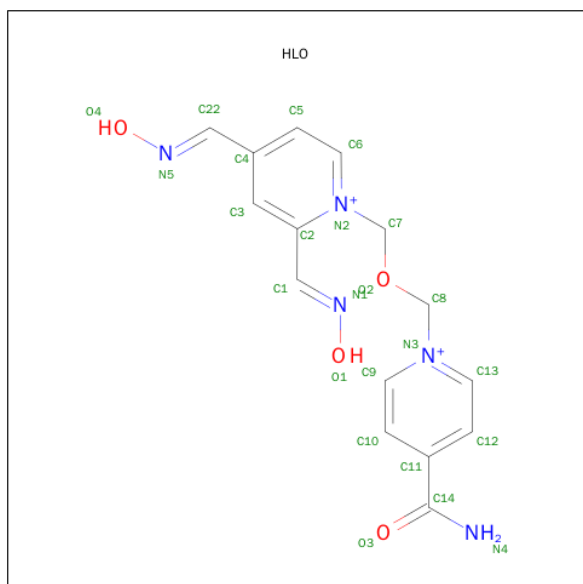
There are 4 unique types of molecules in this entry. The entry contains 8565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	534	Total	C	N	O	S	0	0	1
			4159	2670	719	756	14			

- Molecule 2 is 1-[(2,4-BIS[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL)METHOXY]METHYL-4-CARBAMOYL PYRIDINIUM (three-letter code: HLO) (formula: C₁₅H₁₇N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	15	5	4		
2	B	1	Total	C	N	O	0	0
			24	15	5	4		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	69	Total	O	0	0
			69	69		

Q181	GLY	D333	R424	Q509
G192	GLY	E334	V425	Y510
D193	ALA	G335	Y426	V511
P194	GLY	S336	A427	L518
M195	GLY	Y337	Y428	L524
S196	M265	F338	R433	R525
V197	E268	L339	L437	A526
T198	L269	V340	T438	Q527
L199	L270	Y341	W439	T528
F200	A271	V343	W442	C529
G201	G272	F346	M443	A530
E202	L273	S347	G444	F531
G205	A274	R348	F450	R534
S208	R275	L353	F451	F535
V209	P277	R356	F452	L536
G210	D280	F359	F453	P537
H211	H284	L360	L457	S541
I213	E285	V363	P458	A542
L214	W286	R364	L459	T543
S215	R287	I365	D460	A544
L216	V288	F368	L463	THR
P217	Q291	V379	M464	GLU
S218	I294	L380	Y465	ALA
R219	F295	H381	T466	PRO
G220	R296	Y382	T467	
L221	V300	P391	A473	
F222	P301	R395	L476	
H223	D304	D396	M477	
R224	G305	A397	K478	
V226	D306	M398	Y479	
L227	F307	V401	W480	
Q228	L308	V404	T481	
S229	T311	D404	R485	
G230	P312	H405	T486	
T231	I316	M406	G487	
P232	R317	V407	D491	
A237	G319	V408	P492	
E243	D320	C409	R493	
A244	R247	P410	D494	
R245	K248	V411	S495	
R246	F321	A412	K496	
R247	Q322	Q413	S497	
K248	L249	L417	P498	
T249	L250	L418	Q499	
L251	L251	P501	W500	
A252	A252	F502	P501	
R253	V326	Y503	T504	
L254	L327	G422	T505	
C257	V328	A423		
PRO	G329			
PRO	V330			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.67Å 108.45Å 220.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.70 29.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.88-2.70) 100.0 (29.88-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.261 0.200 , 0.248	Depositor DCC
R_{free} test set	1011 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 51367 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8565	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HLO, P6G

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	0.76	1/4300 (0.0%)	0.78	2/5875 (0.0%)
1	B	0.72	1/4282 (0.0%)	0.77	2/5853 (0.0%)
All	All	0.74	2/8582 (0.0%)	0.77	4/11728 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	413	GLN	CG-CD	6.34	1.65	1.51
1	A	272	CYS	CB-SG	-5.33	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	HIS	N-CA-CB	7.24	123.64	110.60
1	A	287	HIS	N-CA-CB	5.56	120.61	110.60
1	B	216	LEU	CA-CB-CG	-5.30	103.10	115.30
1	A	18	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	4177	0	4065	192	1
1	B	4159	0	4047	188	1
2	A	24	0	17	7	0
2	B	24	0	17	5	0
3	B	19	0	24	8	0
4	A	93	0	0	12	0
4	B	69	0	0	6	0
All	All	8565	0	8170	380	1

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 23.

All (380) 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:197:VAL:H	1:B:223:HIS:CD2	1.75	1.03
1:B:452:GLU:HG3	4:B:2049:HOH:O	1.57	1.02
1:B:497:SER:HB2	1:B:498:PRO:CA	1.89	1.02
1:A:380:LEU:HB3	3:B:1546:P6G:H61	1.43	1.01
1:B:284:HIS:ND1	1:B:287:HIS:CE1	2.31	0.98
1:A:197:VAL:H	1:A:223:HIS:CD2	1.82	0.96
1:B:197:VAL:H	1:B:223:HIS:HD2	0.95	0.95
1:B:497:SER:HB2	1:B:498:PRO:HA	1.49	0.92
1:B:525:ARG:HH11	1:B:525:ARG:HG3	1.37	0.90
1:A:197:VAL:H	1:A:223:HIS:HD2	0.95	0.89
1:A:360:LEU:HD23	1:A:379:VAL:HG21	1.56	0.88
1:B:284:HIS:CG	1:B:287:HIS:CE1	2.62	0.88
1:B:119:TYR:HB2	4:B:2020:HOH:O	1.73	0.86
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.59	0.84
1:A:369:GLN:HB2	4:A:2056:HOH:O	1.77	0.83
1:B:197:VAL:N	1:B:223:HIS:HD2	1.77	0.82
1:B:479:TYR:OH	1:B:518:LEU:HD11	1.80	0.81
1:B:284:HIS:ND1	1:B:287:HIS:NE2	2.28	0.81
1:B:525:ARG:CG	1:B:525:ARG:HH11	1.94	0.81
1:A:213:ILE:O	1:A:219:ARG:HD3	1.79	0.80
1:B:360:LEU:HD22	1:B:379:VAL:HG11	1.64	0.80
1:B:497:SER:HB2	1:B:498:PRO:C	2.02	0.79
1:A:341:TYR:CD2	2:A:1543:HLO:H7C2	2.18	0.78
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.66	0.77
1:B:328:VAL:O	1:B:427:ALA:HA	1.86	0.76
1:A:128:ALA:HB1	1:A:148:SER:HB2	1.68	0.75
1:B:294:ILE:HG12	1:B:365:ILE:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TRP:CH2	2:A:1543:HLO:H8C2	2.23	0.73
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.71	0.73
1:A:287:HIS:HB3	4:A:2053:HOH:O	1.90	0.72
1:B:284:HIS:CG	1:B:287:HIS:HE1	2.08	0.71
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.72	0.71
1:B:112:THR:HG21	1:B:143:GLY:O	1.90	0.71
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.73	0.71
1:B:326:VAL:HG21	1:B:418:LEU:HD13	1.73	0.70
1:A:380:LEU:HB3	3:B:1546:P6G:C6	2.20	0.70
1:B:525:ARG:NH1	1:B:525:ARG:HG3	2.06	0.70
1:B:304:ASP:OD2	1:B:306:ASP:HB3	1.91	0.70
1:A:245:ARG:O	1:A:249:THR:CG2	2.40	0.69
1:A:340:VAL:HG11	1:A:443:MET:CE	2.23	0.69
1:B:80:PHE:CE1	1:B:438:THR:OG1	2.47	0.68
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.24	0.68
1:B:45:ARG:O	1:B:48:MET:HB2	1.93	0.68
1:A:116:ILE:HD12	1:A:197:VAL:HG13	1.76	0.67
1:A:203:SER:HB2	1:A:447:HIS:NE2	2.10	0.66
1:B:433:ARG:NH2	1:B:439:TRP:O	2.28	0.66
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.78	0.66
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.76	0.66
1:A:253:ARG:HD3	4:A:2045:HOH:O	1.95	0.66
1:A:321:PHE:HB2	1:A:423:ALA:HB2	1.78	0.66
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.77	0.65
1:B:322:GLN:HA	1:B:422:GLY:O	1.96	0.65
1:A:116:ILE:HD12	1:A:197:VAL:CG1	2.27	0.64
1:B:277:PRO:HG2	1:B:280:ASP:OD2	1.98	0.64
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.80	0.64
1:A:197:VAL:N	1:A:223:HIS:HD2	1.81	0.64
1:A:294:ILE:HD11	1:A:402:VAL:HG21	1.79	0.64
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.28	0.64
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.79	0.64
1:A:424:ARG:HD2	4:A:2073:HOH:O	1.99	0.63
1:A:122:GLY:O	1:A:123:PHE:HB2	1.99	0.63
1:A:245:ARG:O	1:A:249:THR:HG22	1.99	0.63
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.81	0.63
1:A:160:ALA:HB2	1:A:169:GLY:HA3	1.81	0.62
1:B:497:SER:CB	1:B:498:PRO:HA	2.26	0.62
1:A:341:TYR:CE2	2:A:1543:HLO:H7C2	2.33	0.62
1:B:141:VAL:HG21	1:B:459:LEU:CD2	2.30	0.62
1:A:101:VAL:HG22	1:A:147:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:CG1	1:A:443:MET:HE2	2.30	0.62
1:A:202:GLU:HA	1:A:228:GLN:O	1.99	0.62
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.81	0.62
1:A:527:GLN:HE21	3:B:1546:P6G:H182	1.64	0.61
1:B:250:LEU:HG	1:B:288:VAL:HG12	1.82	0.61
1:B:497:SER:CB	1:B:498:PRO:CA	2.74	0.61
1:A:340:VAL:HG11	1:A:443:MET:HE2	1.81	0.61
1:A:45:ARG:HH22	1:A:54:ARG:HH22	1.47	0.61
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.83	0.61
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.35	0.60
1:B:180:LEU:HB3	1:B:221:LEU:HB3	1.83	0.60
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.35	0.59
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.83	0.59
1:B:45:ARG:NH1	1:B:51:GLU:HG2	2.17	0.59
1:B:101:VAL:HG22	1:B:147:VAL:HG22	1.82	0.59
1:B:285:GLU:O	1:B:288:VAL:HG22	2.02	0.59
1:B:103:THR:HG22	1:B:145:VAL:HG22	1.85	0.59
1:A:470:ARG:O	1:A:474:GLN:HG2	2.03	0.59
1:A:176:GLN:OE1	1:A:208:SER:HB3	2.02	0.59
1:A:245:ARG:O	1:A:249:THR:HG23	2.02	0.59
1:B:74:ASP:HB2	4:B:2018:HOH:O	2.03	0.58
1:A:393:HIS:HD2	4:A:2071:HOH:O	1.87	0.58
1:B:45:ARG:HH11	1:B:51:GLU:HG2	1.67	0.58
1:A:77:TYR:CZ	1:A:348:LYS:HG2	2.38	0.58
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.38	0.58
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.86	0.58
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.86	0.57
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.86	0.57
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.85	0.57
1:B:254:LEU:HD13	1:B:287:HIS:ND1	2.20	0.57
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.40	0.57
1:B:211:MET:HG3	1:B:232:PRO:HB3	1.87	0.57
1:A:85:MET:HE3	1:A:132:VAL:HG11	1.87	0.57
1:B:88:PRO:HG3	1:B:92:LEU:HD21	1.86	0.56
1:A:128:ALA:HB1	1:A:148:SER:CB	2.36	0.56
1:A:17:LEU:HD23	1:A:60:LEU:HB3	1.88	0.56
2:B:1545:HLO:H13	2:B:1545:HLO:H1	1.86	0.56
1:A:271:ALA:O	1:A:275:THR:HG23	2.06	0.56
1:A:46:ARG:HB3	1:A:274:ARG:HG2	1.87	0.56
1:B:200:PHE:CB	1:B:226:VAL:HB	2.35	0.56
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:PRO:O	1:B:541:SER:HB3	2.05	0.56
1:B:511:VAL:HG11	1:B:518:LEU:HD23	1.88	0.56
1:B:265:ASN:ND2	4:B:2035:HOH:O	2.39	0.56
1:B:319:GLY:O	1:B:421:GLN:HG2	2.06	0.56
1:B:96:CYS:O	1:B:150:ASN:HB2	2.06	0.55
1:B:509:GLN:HB2	4:B:2058:HOH:O	2.05	0.55
1:B:341:TYR:CE2	2:B:1545:HLO:H7C2	2.40	0.55
1:A:542:ALA:HB1	1:B:544:ALA:N	2.22	0.55
1:B:224:ARG:HD3	1:B:487:GLY:CA	2.37	0.55
1:A:116:ILE:HD13	1:A:180:LEU:HD22	1.88	0.54
1:A:294:ILE:HD11	1:A:402:VAL:CG2	2.37	0.54
1:A:360:LEU:HD21	1:A:379:VAL:HG11	1.89	0.54
1:A:387:HIS:HB3	1:A:390:ASP:HB2	1.89	0.54
1:A:206:ALA:HB3	1:A:230:GLY:HA3	1.89	0.54
1:B:381:HIS:HA	3:B:1546:P6G:H171	1.89	0.54
1:A:112:THR:HG21	1:A:143:GLY:O	2.08	0.54
1:B:341:TYR:CD2	2:B:1545:HLO:H7C2	2.42	0.54
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.90	0.54
1:A:50:PRO:HB2	1:A:178:LEU:HD22	1.90	0.54
1:B:497:SER:HB3	1:B:499:GLN:HE21	1.73	0.54
1:B:473:ALA:O	1:B:477:MET:HG3	2.07	0.54
1:A:200:PHE:CB	1:A:226:VAL:HB	2.38	0.54
1:A:235:PRO:HG3	1:A:405:HIS:CE1	2.43	0.53
1:A:450:GLU:N	1:A:450:GLU:OE1	2.37	0.53
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.43	0.53
1:B:316:ILE:O	1:B:421:GLN:NE2	2.41	0.53
1:A:328:VAL:O	1:A:427:ALA:HA	2.08	0.53
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.89	0.53
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.89	0.53
1:B:22:LEU:HB3	1:B:136:ARG:HH21	1.73	0.53
1:A:527:GLN:HG3	3:B:1546:P6G:H182	1.90	0.53
1:B:172:GLY:O	1:B:176:GLN:HG3	2.08	0.53
1:B:31:ALA:HB1	1:B:33:LEU:HD21	1.89	0.53
1:A:107:ARG:HD2	1:A:190:PHE:HA	1.90	0.53
1:A:3:ARG:HH11	1:A:3:ARG:HA	1.73	0.53
1:B:535:PHE:CD2	3:B:1546:P6G:H82	2.43	0.53
1:A:340:VAL:HG11	1:A:443:MET:HE1	1.91	0.53
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.91	0.53
1:A:339:LEU:HD11	1:A:399:SER:HA	1.90	0.52
1:A:524:LEU:O	1:A:525:ARG:C	2.48	0.52
1:A:139:ALA:HA	1:A:144:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.45	0.52
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.74	0.52
1:B:404:ASP:HA	1:B:408:VAL:HB	1.90	0.52
1:A:16:GLN:HG2	4:A:2002:HOH:O	2.08	0.52
1:A:231:THR:HB	1:A:233:ASN:OD1	2.10	0.52
1:B:284:HIS:HD1	1:B:287:HIS:HE2	1.57	0.51
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.92	0.51
1:A:541:SER:O	1:A:542:ALA:CB	2.58	0.51
1:B:252:ALA:HA	1:B:273:LEU:HD21	1.92	0.51
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.92	0.51
1:B:36:PRO:HB2	1:B:53:LYS:HD3	1.91	0.51
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.40	0.51
1:B:254:LEU:HD22	1:B:287:HIS:ND1	2.26	0.51
1:A:274:ARG:HD3	4:A:2047:HOH:O	2.09	0.51
1:B:501:PRO:HG2	1:B:509:GLN:HB3	1.92	0.51
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.40	0.51
1:A:38:ALA:HB2	1:A:178:LEU:HD23	1.92	0.51
1:A:20:ILE:HG23	1:A:31:ALA:HB3	1.93	0.51
1:A:210:GLY:HA2	1:A:213:ILE:HD12	1.93	0.51
1:A:540:LEU:O	1:A:542:ALA:N	2.41	0.50
1:B:382:TYR:CD1	1:B:401:VAL:HG22	2.46	0.50
1:A:96:CYS:O	1:A:150:ASN:HB2	2.10	0.50
1:B:99:LEU:HA	1:B:149:MET:HA	1.93	0.50
1:A:316:ILE:O	1:A:421:GLN:NE2	2.45	0.49
1:A:100:ASN:O	1:A:147:VAL:HA	2.12	0.49
1:A:249:THR:O	1:A:252:ALA:HB3	2.12	0.49
1:B:48:MET:SD	1:B:166:GLU:HA	2.52	0.49
1:B:30:SER:HB2	1:B:103:THR:OG1	2.12	0.49
1:A:3:ARG:NH1	1:A:3:ARG:HG3	2.28	0.49
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.48	0.49
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.93	0.49
1:A:142:GLU:CB	1:A:481:THR:HG21	2.43	0.49
1:A:395:ARG:CZ	1:A:442:TRP:HB2	2.43	0.49
1:A:374:ALA:HB1	1:A:536:LEU:HD21	1.95	0.48
1:B:327:LEU:HD11	1:B:500:TRP:CH2	2.48	0.48
1:B:527:GLN:O	1:B:530:ALA:HB3	2.13	0.48
1:A:339:LEU:HD11	1:A:399:SER:CA	2.42	0.48
1:B:202:GLU:HA	1:B:228:GLN:O	2.12	0.48
1:A:77:TYR:CE1	1:A:348:LYS:HG2	2.48	0.48
1:A:46:ARG:NH1	1:A:276:ARG:O	2.41	0.48
1:A:22:LEU:HB2	1:A:29:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PHE:O	1:B:363:VAL:HG23	2.14	0.48
1:B:158:PHE:HE1	1:B:173:LEU:HG	1.78	0.48
1:B:237:ALA:O	1:B:301:PRO:HD2	2.14	0.48
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.95	0.48
1:A:84:GLU:OE1	1:A:84:GLU:HA	2.13	0.48
1:A:393:HIS:CD2	4:A:2071:HOH:O	2.62	0.48
1:A:414:LEU:O	1:A:418:LEU:HB2	2.14	0.47
1:B:146:LEU:HD23	1:B:147:VAL:N	2.29	0.47
1:B:479:TYR:OH	1:B:518:LEU:CD1	2.58	0.47
1:A:504:THR:O	1:A:508:GLN:N	2.39	0.47
1:B:243:GLU:O	1:B:247:ARG:HG3	2.15	0.47
1:A:282:VAL:O	1:A:285:GLU:HG2	2.14	0.47
1:B:89:ASN:O	1:B:90:ARG:NH1	2.45	0.47
1:A:536:LEU:N	1:A:537:PRO:CD	2.78	0.47
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.71	0.47
1:A:525:ARG:HD3	4:A:2087:HOH:O	2.15	0.47
1:A:181:GLN:O	1:A:184:GLN:HB2	2.15	0.47
1:A:341:TYR:CD2	2:A:1543:HLO:C7	2.94	0.47
1:B:493:ARG:O	1:B:494:ASP:HB2	2.14	0.47
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.95	0.47
1:B:330:VAL:HG11	1:B:408:VAL:HA	1.96	0.47
1:A:352:SER:O	1:A:395:ARG:HG3	2.15	0.47
1:B:161:LEU:HD12	1:B:270:ILE:HG13	1.96	0.47
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.48	0.47
1:A:120:GLY:HA2	1:A:205:GLY:H	1.80	0.47
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.97	0.47
1:A:77:TYR:CG	1:A:348:LYS:HD3	2.50	0.47
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.46	0.46
1:A:80:PHE:CE1	1:A:348:LYS:HE3	2.50	0.46
1:A:407:VAL:C	1:A:410:PRO:HD2	2.35	0.46
1:A:116:ILE:CD1	1:A:197:VAL:HG13	2.44	0.46
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.51	0.46
1:B:271:ALA:O	1:B:274:ARG:HB2	2.15	0.46
1:A:430:PHE:CD2	1:A:450:GLU:HB2	2.51	0.46
1:B:518:LEU:HD12	4:B:2061:HOH:O	2.15	0.46
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.45	0.46
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.15	0.46
1:A:330:VAL:HG11	1:A:408:VAL:HA	1.98	0.46
1:A:287:HIS:CB	4:A:2053:HOH:O	2.57	0.46
1:A:33:LEU:HD22	1:A:65:PHE:CE1	2.50	0.46
1:A:397:ALA:O	1:A:401:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD11	1:A:225:ALA:CB	2.45	0.45
1:B:339:LEU:O	1:B:343:VAL:HB	2.15	0.45
1:A:528:THR:O	1:A:531:PHE:HB3	2.16	0.45
1:A:80:PHE:O	1:A:84:GLU:HG2	2.16	0.45
1:A:537:PRO:O	1:A:540:LEU:HD23	2.17	0.45
1:B:214:LEU:HD11	1:B:316:ILE:HG23	1.98	0.45
1:B:317:ASN:HA	1:B:417:ARG:HH11	1.82	0.45
1:A:428:TYR:HB3	1:A:500:TRP:CZ2	2.51	0.45
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.98	0.45
1:A:70:TYR:HD2	1:A:282:VAL:HG21	1.80	0.45
1:B:528:THR:O	1:B:531:PHE:HB3	2.16	0.45
1:A:380:LEU:HD11	1:B:534:ARG:HB2	1.98	0.45
1:A:374:ALA:HA	1:A:539:LEU:HD23	1.98	0.45
1:A:7:GLN:HG2	4:A:2023:HOH:O	2.16	0.45
1:A:334:GLU:CD	1:A:407:VAL:HG11	2.37	0.45
1:B:525:ARG:NH1	1:B:525:ARG:CG	2.63	0.45
1:B:22:LEU:HD13	1:B:136:ARG:NH2	2.32	0.45
1:A:485:ARG:HB3	1:A:486:THR:HG23	1.99	0.45
1:A:9:LEU:HB3	4:A:2002:HOH:O	2.17	0.45
2:A:1543:HLO:H8C1	2:A:1543:HLO:C1	2.47	0.44
1:A:321:PHE:CB	1:A:423:ALA:HB2	2.44	0.44
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.98	0.44
1:A:339:LEU:HD11	1:A:399:SER:N	2.32	0.44
1:B:542:ALA:O	1:B:543:THR:OG1	2.30	0.44
1:A:333:ASP:O	1:A:446:PRO:HA	2.16	0.44
1:B:346:PHE:HE2	1:B:395:ARG:HG2	1.81	0.44
1:B:382:TYR:HB3	1:B:397:ALA:HB1	1.99	0.44
1:B:317:ASN:HA	1:B:417:ARG:NH1	2.33	0.44
1:B:213:ILE:O	1:B:219:ARG:HD3	2.16	0.44
1:A:183:VAL:HG13	1:A:187:ILE:HB	1.98	0.44
1:B:193:ASP:C	1:B:195:MET:H	2.20	0.44
1:B:105:TYR:C	1:B:105:TYR:CD2	2.90	0.44
1:B:499:GLN:O	1:B:501:PRO:HD3	2.16	0.44
1:B:53:LYS:HG3	1:B:54:ARG:O	2.17	0.44
1:A:356:ARG:NH2	1:A:383:THR:OG1	2.43	0.44
1:A:1:GLU:N	1:A:4:GLU:OE1	2.42	0.44
1:A:294:ILE:CD1	1:A:402:VAL:HG21	2.47	0.44
1:B:120:GLY:HA2	1:B:205:GLY:H	1.83	0.44
1:A:527:GLN:HG3	3:B:1546:P6G:C18	2.48	0.43
1:A:310:ASP:OD1	1:A:311:THR:N	2.45	0.43
1:A:479:TYR:OH	1:A:518:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:O	1:B:249:THR:OG1	2.24	0.43
1:B:498:PRO:HG2	1:B:518:LEU:O	2.18	0.43
1:B:338:PHE:CE2	2:B:1545:HLO:H3	2.52	0.43
1:B:333:ASP:O	1:B:334:GLU:C	2.56	0.43
1:B:284:HIS:CB	1:B:287:HIS:CE1	3.00	0.43
1:B:407:VAL:C	1:B:410:PRO:HD2	2.38	0.43
1:B:20:ILE:HB	1:B:63:THR:HB	2.00	0.43
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.54	0.43
1:B:336:SER:O	1:B:337:TYR:C	2.57	0.43
1:A:474:GLN:HE21	1:A:474:GLN:HB3	1.62	0.43
1:B:340:VAL:CG1	1:B:443:MET:CE	2.97	0.43
1:B:428:TYR:HA	1:B:511:VAL:O	2.18	0.43
1:A:381:HIS:HA	3:B:1546:P6G:H31	2.00	0.43
1:A:430:PHE:HE2	1:A:476:LEU:CD1	2.31	0.43
1:A:202:GLU:OE2	1:A:448:GLY:HA2	2.18	0.43
1:B:146:LEU:HD23	1:B:146:LEU:C	2.39	0.43
1:B:202:GLU:HG3	1:B:450:GLU:OE2	2.19	0.43
1:B:68:VAL:CG1	1:B:71:GLN:NE2	2.82	0.43
1:B:36:PRO:HD3	1:B:60:LEU:HD21	2.01	0.43
1:B:132:VAL:HG12	1:B:452:GLU:HG2	2.00	0.43
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.79	0.43
1:A:380:LEU:HD11	1:B:534:ARG:CB	2.49	0.42
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.84	0.42
1:A:321:PHE:O	1:A:423:ALA:HA	2.19	0.42
1:A:541:SER:O	1:A:542:ALA:HB3	2.19	0.42
1:A:235:PRO:HB2	1:A:296:ARG:NH2	2.34	0.42
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.54	0.42
1:B:35:ILE:O	1:B:98:TYR:HA	2.19	0.42
1:B:425:VAL:O	1:B:503:TYR:N	2.52	0.42
1:A:116:ILE:HA	1:A:147:VAL:O	2.19	0.42
1:B:326:VAL:HG21	1:B:418:LEU:CD1	2.45	0.42
1:B:166:GLU:CB	1:B:274:ARG:HH22	2.32	0.42
1:A:226:VAL:HA	1:A:327:LEU:O	2.18	0.42
1:A:335:GLY:HA3	1:A:399:SER:O	2.18	0.42
1:B:321:PHE:HB3	1:B:423:ALA:HB2	2.02	0.42
1:A:39:GLU:O	1:A:40:PRO:C	2.57	0.42
1:A:173:LEU:HB3	1:A:307:PHE:CZ	2.55	0.42
1:B:231:THR:HG21	1:B:411:VAL:HA	2.01	0.42
1:B:433:ARG:HG3	1:B:444:GLY:O	2.19	0.42
1:B:124:TYR:C	1:B:124:TYR:CD1	2.93	0.42
1:A:209:VAL:CG1	1:A:225:ALA:HB1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1543:HLO:H1	2:A:1543:HLO:C13	2.49	0.42
1:A:232:PRO:HD2	1:A:414:LEU:HD13	2.02	0.42
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.01	0.42
1:A:382:TYR:CD1	1:A:401:VAL:HG22	2.54	0.42
1:B:398:MET:HA	1:B:398:MET:HE3	2.02	0.42
1:A:88:PRO:CG	1:A:92:LEU:HD21	2.50	0.42
1:B:117:TRP:HA	1:B:200:PHE:O	2.20	0.42
1:B:214:LEU:HD21	1:B:316:ILE:HG22	2.02	0.42
1:A:117:TRP:CZ3	1:A:201:GLY:HA2	2.55	0.42
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.55	0.42
1:B:80:PHE:CD1	1:B:348:LYS:HE2	2.55	0.41
1:A:327:LEU:HD11	1:A:500:TRP:CZ2	2.55	0.41
1:B:364:ARG:O	1:B:368:PRO:HA	2.20	0.41
1:A:376:GLU:OE2	1:A:380:LEU:CD2	2.68	0.41
1:A:309:SER:OG	1:A:315:LEU:HD21	2.20	0.41
1:A:30:SER:HB2	1:A:103:THR:OG1	2.20	0.41
1:B:22:LEU:HB2	1:B:29:VAL:HG23	2.02	0.41
1:A:525:ARG:O	1:A:526:ALA:C	2.57	0.41
1:B:311:THR:O	1:B:312:PRO:C	2.58	0.41
1:B:85:MET:CE	1:B:132:VAL:HG11	2.50	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.20	0.41
1:B:276:ARG:O	1:B:277:PRO:C	2.59	0.41
1:B:89:ASN:O	1:B:90:ARG:HG2	2.21	0.41
1:A:224:ARG:HD3	1:A:487:GLY:CA	2.50	0.41
1:A:346:PHE:HE2	1:A:395:ARG:HG2	1.86	0.41
1:B:107:ARG:HE	1:B:107:ARG:HB2	1.38	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CD2	2.55	0.41
1:A:60:LEU:HD23	1:A:61:ASP:C	2.41	0.41
1:B:284:HIS:CE1	1:B:287:HIS:CE1	3.05	0.41
1:B:134:ASP:OD2	1:B:136:ARG:HD2	2.20	0.41
1:A:233:ASN:OD1	1:A:233:ASN:N	2.52	0.41
1:B:177:ARG:CZ	1:B:307:PHE:CE2	3.03	0.41
1:A:497:SER:HA	1:A:498:PRO:HD3	1.94	0.41
1:B:251:LEU:HA	1:B:254:LEU:HD12	2.03	0.41
1:B:453:PHE:HB3	1:B:476:LEU:CD1	2.51	0.41
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.84	0.41
1:B:295:PHE:CE2	1:B:338:PHE:CE1	3.09	0.41
1:A:199:LEU:O	1:A:226:VAL:N	2.49	0.41
1:A:293:SER:CB	1:A:296:ARG:HB2	2.51	0.41
1:A:3:ARG:HH11	1:A:3:ARG:CG	2.34	0.41
1:A:142:GLU:HB3	1:A:481:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:O	1:A:447:HIS:HE1	2.04	0.41
1:B:340:VAL:HG11	1:B:443:MET:CE	2.51	0.41
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.56	0.41
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.51	0.41
1:B:145:VAL:HG21	1:B:192:GLY:CA	2.52	0.40
1:A:208:SER:O	1:A:209:VAL:C	2.57	0.40
1:A:85:MET:HE3	1:A:132:VAL:CG1	2.51	0.40
1:B:76:LEU:HD22	1:B:341:TYR:CD2	2.56	0.40
1:B:199:LEU:O	1:B:226:VAL:N	2.54	0.40
1:B:36:PRO:CD	1:B:60:LEU:HD21	2.52	0.40
1:B:229:SER:OG	1:B:334:GLU:OE2	2.27	0.40
1:A:130:LEU:HB2	1:A:133:TYR:CD2	2.56	0.40
1:B:142:GLU:HB3	1:B:481:THR:HG21	2.02	0.40
2:A:1543:HLO:H1	2:A:1543:HLO:H13	2.03	0.40
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.03	0.40
1:A:47:PHE:CE2	1:A:273:LEU:HB3	2.57	0.40
1:B:457:LEU:N	1:B:458:PRO:CD	2.85	0.40
1:A:525:ARG:HB2	1:A:529:CYS:SG	2.62	0.40
1:B:177:ARG:NH2	1:B:307:PHE:CE2	2.89	0.40
1:A:385:TRP:CD1	1:B:530:ALA:HB2	2.57	0.40
1:A:365:ILE:O	1:A:368:PRO:HD3	2.21	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.83	0.40
1:A:123:PHE:O	1:A:154:GLY:N	2.29	0.40
1:A:56:TRP:NE1	1:A:60:LEU:HB2	2.36	0.40
1:B:338:PHE:HE2	2:B:1545:HLO:H3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH1	1:B:57:SER:O[2_555]	2.14	0.06

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	531/548 (97%)	491 (92%)	37 (7%)	3 (1%)	30	59
1	B	530/548 (97%)	492 (93%)	33 (6%)	5 (1%)	21	49
All	All	1061/1096 (97%)	983 (93%)	70 (7%)	8 (1%)	24	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	497	SER
1	A	541	SER
1	B	541	SER
1	A	493	ARG
1	B	496	LYS
1	B	543	THR
1	A	342	GLY

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	439/446 (98%)	411 (94%)	28 (6%)	22	47
1	B	438/446 (98%)	409 (93%)	29 (7%)	21	45
All	All	877/892 (98%)	820 (94%)	57 (6%)	21	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	GLN
1	A	13	ARG
1	A	23	LYS
1	A	64	THR

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Mol	Chain	Res	Type
1	A	93	SER
1	A	200	PHE
1	A	216	LEU
1	A	246	ARG
1	A	249	THR
1	A	280	ASP
1	A	287	HIS
1	A	291	GLN
1	A	295	PHE
1	A	320	ASP
1	A	322	GLN
1	A	337	TYR
1	A	418	LEU
1	A	421	GLN
1	A	424	ARG
1	A	441	LEU
1	A	471	ILE
1	A	474	GLN
1	A	514	ASN
1	A	519	GLU
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	9	LEU
1	B	23	LYS
1	B	51	GLU
1	B	105	TYR
1	B	107	ARG
1	B	181	GLN
1	B	200	PHE
1	B	216	LEU
1	B	286	TRP
1	B	287	HIS
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	326	VAL
1	B	348	LYS
1	B	356	ARG
1	B	417	ARG
1	B	421	GLN
1	B	437	LEU

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Mol	Chain	Res	Type
1	B	438	THR
1	B	457	LEU
1	B	467	THR
1	B	478	LYS
1	B	496	LYS
1	B	497	SER
1	B	505	THR
1	B	524	LEU
1	B	525	ARG
1	B	536	LEU

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	223	HIS
1	A	291	GLN
1	A	393	HIS
1	A	421	GLN
1	A	464	ASN
1	A	474	GLN
1	B	223	HIS
1	B	291	GLN
1	B	499	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	HLO	A	1543	-	21,25,25	0.69	0	21,32,32	1.91	2 (9%)
2	HLO	B	1545	-	21,25,25	0.66	0	21,32,32	2.20	2 (9%)
3	P6G	B	1546	-	18,18,18	1.75	5 (27%)	17,17,17	1.97	8 (47%)

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	HLO	A	1543	-	-	0/15/16/16	0/2/2/2
2	HLO	B	1545	-	-	0/15/16/16	0/2/2/2
3	P6G	B	1546	-	-	0/16/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1546	P6G	C9-C8	-3.05	1.33	1.48
3	B	1546	P6G	C17-C18	-2.86	1.33	1.49
3	B	1546	P6G	C15-C14	-2.85	1.34	1.48
3	B	1546	P6G	C6-C5	-2.85	1.34	1.48
3	B	1546	P6G	C3-C2	-2.80	1.33	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1546	P6G	O4-C5-C6	2.10	119.70	110.36
3	B	1546	P6G	C8-O7-C6	2.16	122.58	113.31
3	B	1546	P6G	O4-C3-C2	2.16	120.39	110.43
3	B	1546	P6G	C5-O4-C3	2.21	122.81	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	1546	P6G	O7-C8-C9	2.26	120.41	110.36
3	B	1546	P6G	O7-C6-C5	2.28	120.51	110.36
3	B	1546	P6G	O16-C15-C14	2.87	123.12	110.36
3	B	1546	P6G	O13-C14-C15	3.48	125.82	110.36
2	A	1543	HLO	O1-N1-C1	3.98	118.67	111.88
2	B	1545	HLO	O1-N1-C1	5.79	121.75	111.88
2	A	1543	HLO	O4-N5-C22	6.71	123.32	111.88
2	B	1545	HLO	O4-N5-C22	7.38	124.46	111.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1543	HLO	7	0
2	B	1545	HLO	5	0
3	B	1546	P6G	8	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	535/548 (97%)	-0.15	13 (2%) 62 62	19, 34, 55, 78	0
1	B	534/548 (97%)	-0.08	14 (2%) 59 59	23, 38, 57, 75	0
All	All	1069/1096 (97%)	-0.11	27 (2%) 61 61	19, 36, 56, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	7.3
1	A	496	LYS	4.3
1	A	203	SER	3.5
1	A	493	ARG	3.4
1	B	78	PRO	3.4
1	B	543	THR	3.2
1	B	79	GLY	3.2
1	B	497	SER	3.1
1	B	495	SER	3.0
1	B	496	LYS	2.9
1	B	268	GLU	2.8
1	A	540	LEU	2.8
1	A	206	ALA	2.6
1	B	492	PRO	2.6
1	A	287	HIS	2.5
1	A	497	SER	2.4
1	A	165	ARG	2.4
1	B	323	ASP	2.3
1	A	201	GLY	2.3
1	B	493	ARG	2.2
1	A	76	LEU	2.2
1	B	109	ALA	2.2
1	A	318	THR	2.2
1	B	467	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLN	2.1
1	A	342	GLY	2.1
1	A	322	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HLO	B	1545	24/24	0.92	0.28	3.26	41,51,60,60	24
3	P6G	B	1546	19/19	0.90	0.23	3.01	47,52,62,62	0
2	HLO	A	1543	24/24	0.94	0.19	0.33	32,42,55,58	24

6.5 Other polymers [i](#)

There are no such residues in this entry.