Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:58 AM GMT

PDB ID	:	2OYE
Title	:	Indomethacin-(R)-alpha-ethyl-ethanolamide bound to Cyclooxygenase-1
Authors	:	Harman, C.A.; Garavito, R.M.
Deposited on	:	2007-02-21
Resolution	:	2.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

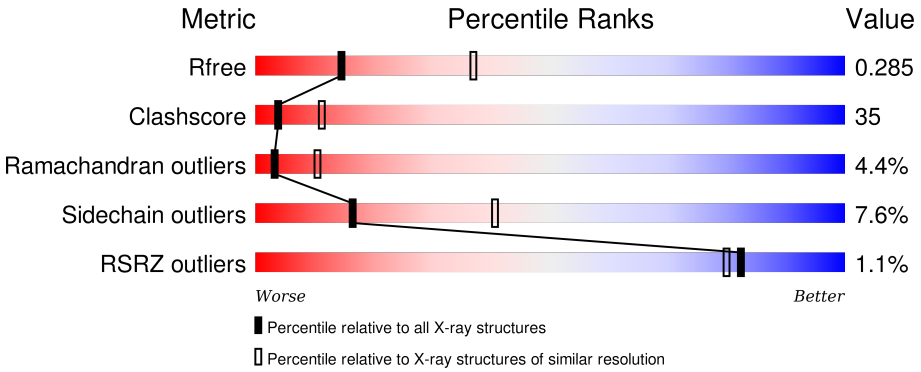
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 <=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	P	600	% 44% 42% 7% • 8%

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
5	BOG	P	751	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4605 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 Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	553	Total	C	N	O	S	0	0	0
			4362	2838	728	768	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	92	LEU	MET	SEE REMARK 999	UNP P05979

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	P	2	Total	C	N	O	0	0
			28	16	2	10		

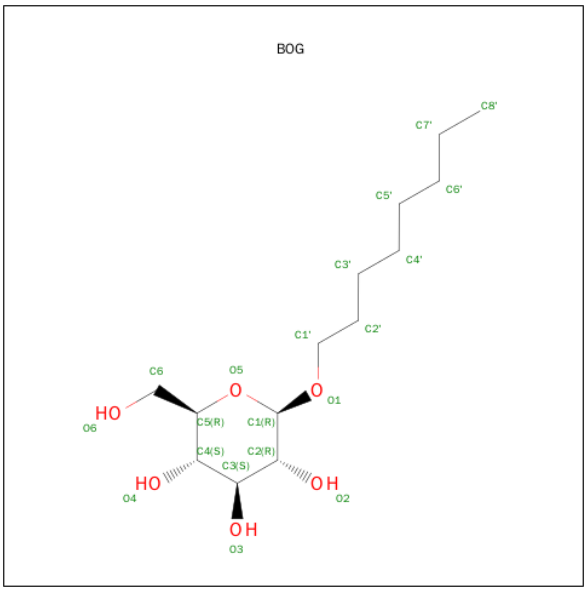
- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

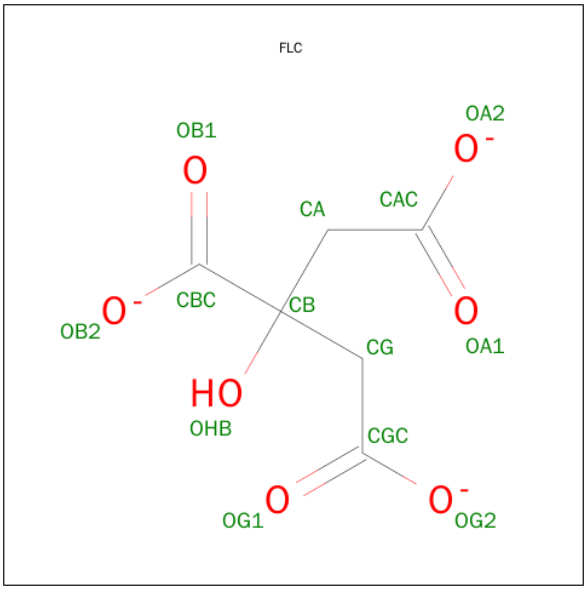
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total C O 12 6 6	0	0
5	P	1	Total C O 12 6 6	0	0

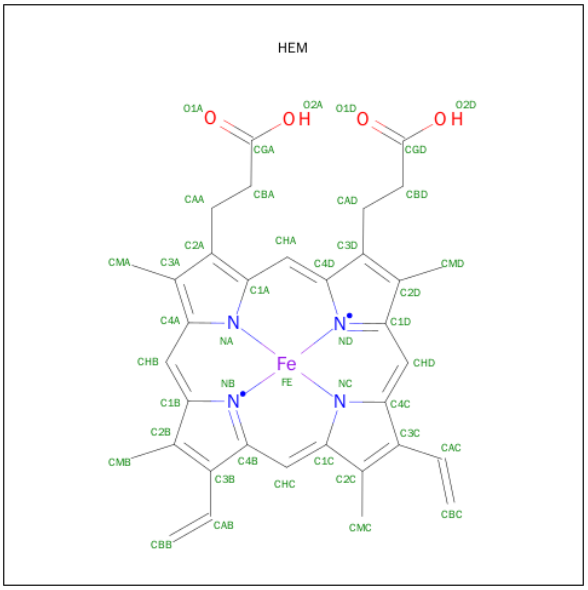
- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total C O 13 6 7	0	0

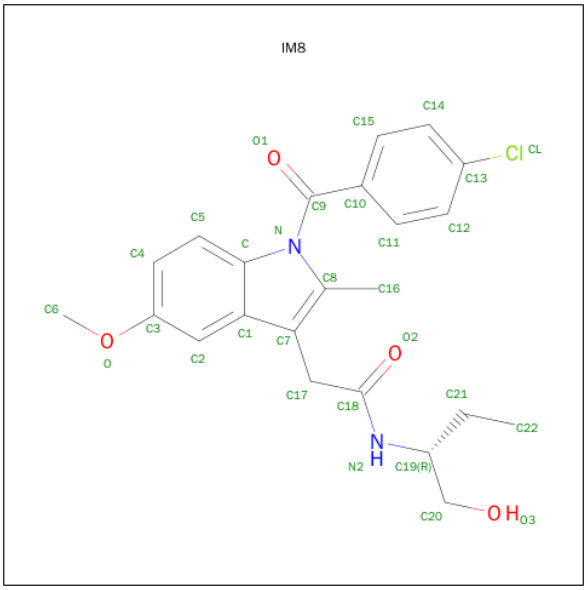
- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is 2-[1-(4-CHLOROBENZOYL)-5-METHOXY-2-METHYL-1H-INDOL-3-YL]-N-[(1R)-1-(HYDROXYMETHYL)PROPYL]ACETAMIDE (three-letter code: IM8) (formula: $C_{23}H_{25}ClN_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	P	1	Total	C	Cl	N	O	0	0
			30	23	1	2	4		

- Molecule 9 is water.

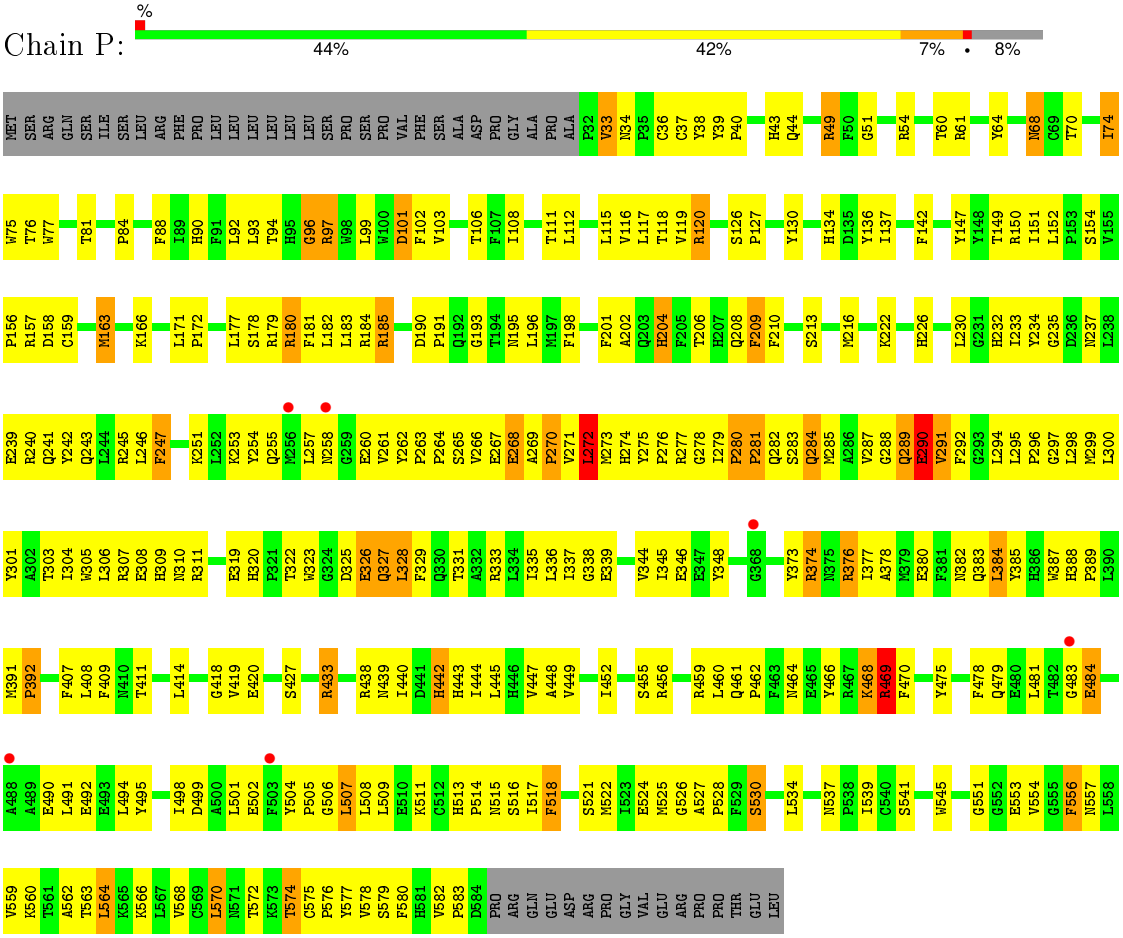
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Prostaglandin G/H synthase 1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.72Å 181.72Å 104.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.85 29.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (30.00-2.85) 89.9 (29.67-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.292 0.243 , 0.285	Depositor DCC
R_{free} test set	950 reflections (4.31%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 26435 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, NDG, HEM, IM8, FLC, BOG

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	P	0.47	0/4501	0.71	1/6136 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	272	LEU	CA-CB-CG	5.84	128.72	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	147	TYR	Sidechain

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	P	4362	0	4159	304	0
2	P	28	0	25	0	0
3	P	50	0	43	4	0
4	P	28	0	25	0	0
5	P	24	0	22	5	0
6	P	13	0	5	3	0
7	P	43	0	30	6	0
8	P	30	0	25	5	0
9	P	27	0	0	5	0
All	All	4605	0	4334	310	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 35.

All (310) 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:P:240:ARG:HG3	1:P:271:VAL:HG21	1.34	1.08
1:P:151:ILE:HG23	1:P:469:ARG:NH1	1.81	0.95
1:P:339:GLU:HG2	1:P:562:ALA:HB2	1.48	0.95
1:P:202:ALA:O	1:P:206:THR:HG23	1.71	0.90
1:P:387:TRP:HB2	7:P:601:HEM:HBC2	1.53	0.90
1:P:182:LEU:HB3	1:P:440:ILE:HD12	1.55	0.89
1:P:391:MET:HG3	7:P:601:HEM:HAB	1.56	0.86
1:P:120:ARG:NH1	8:P:700:IM8:H201	1.93	0.83
1:P:102:PHE:O	1:P:106:THR:HG23	1.79	0.81
1:P:566:LYS:O	1:P:570:LEU:HB2	1.82	0.79
1:P:582:VAL:HG23	1:P:583:PRO:HD2	1.64	0.78
1:P:272:LEU:HD12	1:P:273:MET:N	1.98	0.78
1:P:243:GLN:HG3	1:P:270:PRO:HG2	1.67	0.76
1:P:344:VAL:O	1:P:348:TYR:HB3	1.85	0.76
1:P:241:GLN:O	1:P:245:ARG:HG3	1.86	0.76
1:P:191:PRO:HB2	1:P:515:ASN:HA	1.69	0.75
1:P:216:MET:HG2	3:P:672:NAG:H82	1.70	0.74
1:P:300:LEU:HD11	1:P:419:VAL:HG13	1.70	0.74
1:P:163:MET:HB3	1:P:462:PRO:HG3	1.70	0.73
1:P:388:HIS:HB3	1:P:444:ILE:HD12	1.71	0.73
1:P:137:ILE:HD12	1:P:137:ILE:H	1.53	0.72
1:P:504:TYR:HB3	1:P:505:PRO:HD3	1.70	0.72
1:P:263:PRO:HD2	1:P:285:MET:CE	2.20	0.71
1:P:119:VAL:HG12	5:P:751:BOG:H61	1.74	0.70
1:P:262:TYR:HB3	1:P:285:MET:CE	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:208:GLN:NE2	1:P:230:LEU:H	1.89	0.70
1:P:112:LEU:O	1:P:116:VAL:HG23	1.91	0.70
1:P:326:GLU:OE1	1:P:326:GLU:HA	1.92	0.70
1:P:115:LEU:O	1:P:119:VAL:HG23	1.92	0.69
1:P:530:SER:O	1:P:534:LEU:HD23	1.93	0.69
1:P:208:GLN:HE22	1:P:230:LEU:HD12	1.58	0.69
1:P:237:ASN:ND2	1:P:240:ARG:H	1.91	0.69
1:P:171:LEU:HB2	1:P:456:ARG:NH1	2.09	0.68
1:P:323:TRP:CE3	1:P:327:GLN:HG2	2.29	0.67
1:P:291:VAL:HG22	1:P:294:LEU:HD12	1.75	0.67
1:P:298:LEU:HD12	1:P:298:LEU:N	2.10	0.67
1:P:204:HIS:CD2	1:P:232:HIS:CD2	2.82	0.66
1:P:287:VAL:HG23	1:P:289:GLN:H	1.62	0.65
1:P:183:LEU:HD13	1:P:445:LEU:HD22	1.79	0.65
1:P:156:PRO:HB2	1:P:159:CYS:SG	2.36	0.65
1:P:163:MET:HE1	1:P:460:LEU:O	1.96	0.65
1:P:120:ARG:NH1	8:P:700:IM8:C20	2.60	0.64
1:P:171:LEU:HD12	1:P:456:ARG:HD3	1.77	0.64
1:P:237:ASN:HD21	1:P:240:ARG:H	1.42	0.64
1:P:339:GLU:HG2	1:P:562:ALA:CB	2.26	0.64
1:P:320:HIS:HB3	1:P:323:TRP:CD1	2.33	0.64
1:P:239:GLU:CD	1:P:239:GLU:H	2.01	0.64
1:P:137:ILE:HD12	1:P:137:ILE:N	2.13	0.63
1:P:151:ILE:HG23	1:P:469:ARG:HH11	1.62	0.63
1:P:553:GLU:HG3	1:P:557:ASN:HD21	1.62	0.63
1:P:88:PHE:CE2	1:P:92:LEU:HD11	2.34	0.63
1:P:64:TYR:CE1	1:P:76:THR:HG21	2.34	0.62
1:P:513:HIS:HB2	1:P:516:SER:OG	1.99	0.62
1:P:119:VAL:HG12	5:P:751:BOG:C6	2.29	0.62
1:P:279:ILE:O	1:P:279:ILE:HG22	2.00	0.62
1:P:282:GLN:O	1:P:283:SER:HB2	1.99	0.62
1:P:504:TYR:CZ	1:P:508:LEU:HD11	2.34	0.62
1:P:208:GLN:HE21	1:P:230:LEU:H	1.46	0.62
1:P:242:TYR:CD2	1:P:247:PHE:HZ	2.18	0.62
1:P:185:ARG:N	1:P:185:ARG:HD2	2.15	0.62
1:P:43:HIS:O	1:P:44:GLN:HB2	2.00	0.61
1:P:204:HIS:ND1	1:P:301:TYR:HB3	2.16	0.61
1:P:196:LEU:HD11	1:P:392:PRO:HG3	1.83	0.61
1:P:280:PRO:HA	1:P:284:GLN:CG	2.31	0.60
1:P:333:ARG:O	1:P:337:ILE:HG13	2.02	0.60
1:P:279:ILE:C	1:P:281:PRO:HD2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:134:HIS:HB3	1:P:136:TYR:CE1	2.36	0.60
1:P:260:GLU:CB	1:P:262:TYR:HE1	2.15	0.60
1:P:77:TRP:O	1:P:81:THR:HG23	2.01	0.60
1:P:263:PRO:HB2	1:P:285:MET:HB3	1.84	0.60
1:P:251:LYS:HB3	1:P:310:ASN:ND2	2.17	0.60
1:P:130:TYR:HB2	1:P:150:ARG:HG3	1.83	0.60
1:P:442:HIS:NE2	1:P:443:HIS:CE1	2.70	0.60
1:P:483:GLY:N	1:P:511:LYS:HB3	2.17	0.59
1:P:150:ARG:HD3	1:P:152:LEU:O	2.03	0.59
6:P:900:FLC:HG2	6:P:900:FLC:OA2	2.00	0.59
1:P:263:PRO:HD2	1:P:285:MET:HE1	1.83	0.59
1:P:564:LEU:HD22	1:P:578:VAL:HG21	1.84	0.59
1:P:195:ASN:ND2	1:P:427:SER:HA	2.16	0.59
1:P:563:THR:HG22	1:P:564:LEU:N	2.18	0.59
1:P:40:PRO:O	1:P:68:ASN:HB3	2.03	0.59
1:P:213:SER:HA	1:P:222:LYS:HE2	1.84	0.59
1:P:181:PHE:O	1:P:438:ARG:N	2.36	0.59
1:P:308:GLU:O	1:P:311:ARG:HB3	2.02	0.58
1:P:93:LEU:CD1	8:P:700:IM8:H222	2.34	0.58
1:P:163:MET:HA	1:P:163:MET:CE	2.33	0.58
1:P:275:TYR:CD2	1:P:284:GLN:HG2	2.39	0.58
1:P:388:HIS:HB3	1:P:444:ILE:CD1	2.33	0.58
1:P:126:SER:HA	1:P:127:PRO:C	2.24	0.58
1:P:344:VAL:HG11	1:P:534:LEU:HD11	1.86	0.57
1:P:464:ASN:HB3	9:P:903:HOH:O	2.04	0.57
1:P:295:LEU:CD2	7:P:601:HEM:HBB2	2.35	0.57
1:P:204:HIS:CD2	1:P:232:HIS:HD2	2.22	0.57
1:P:269:ALA:O	1:P:271:VAL:N	2.35	0.57
1:P:263:PRO:HD2	1:P:285:MET:HE2	1.87	0.57
1:P:442:HIS:CD2	1:P:443:HIS:N	2.73	0.57
1:P:568:VAL:O	1:P:572:THR:HG23	2.05	0.57
1:P:553:GLU:HG3	1:P:557:ASN:ND2	2.19	0.56
1:P:527:ALA:HB3	1:P:528:PRO:HD3	1.86	0.56
1:P:537:ASN:OD1	1:P:539:ILE:HG23	2.06	0.56
6:P:900:FLC:HA1	7:P:601:HEM:HAA1	1.88	0.56
1:P:196:LEU:HD21	1:P:392:PRO:HD3	1.85	0.56
1:P:577:TYR:CE2	1:P:583:PRO:HD3	2.41	0.56
1:P:246:LEU:HD12	1:P:253:LYS:HG2	1.88	0.56
1:P:97:ARG:O	1:P:101:ASP:OD2	2.24	0.56
6:P:900:FLC:CA	7:P:601:HEM:HAA1	2.36	0.56
1:P:448:ALA:O	1:P:452:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:177:LEU:HD12	1:P:181:PHE:CE1	2.41	0.56
1:P:237:ASN:OD1	1:P:240:ARG:HB2	2.06	0.56
1:P:234:TYR:CE2	1:P:333:ARG:HG3	2.41	0.55
1:P:468:LYS:O	1:P:470:PHE:N	2.39	0.55
1:P:245:ARG:NH2	1:P:325:ASP:OD2	2.39	0.55
1:P:479:GLN:CB	9:P:923:HOH:O	2.55	0.55
1:P:103:VAL:HG13	1:P:108:ILE:HB	1.88	0.55
1:P:564:LEU:HD13	1:P:578:VAL:HG22	1.88	0.55
1:P:297:GLY:O	1:P:300:LEU:HB3	2.06	0.55
3:P:673:BMA:H61	9:P:925:HOH:O	2.06	0.55
1:P:120:ARG:HE	5:P:751:BOG:H62	1.71	0.55
1:P:309:HIS:CD2	1:P:309:HIS:C	2.79	0.55
1:P:442:HIS:HD2	1:P:443:HIS:N	2.05	0.55
1:P:142:PHE:O	1:P:376:ARG:NH2	2.40	0.55
1:P:388:HIS:N	1:P:389:PRO:HD2	2.21	0.54
1:P:327:GLN:O	1:P:329:PHE:N	2.40	0.54
1:P:279:ILE:C	1:P:281:PRO:CD	2.76	0.54
1:P:172:PRO:HB2	1:P:177:LEU:HD22	1.89	0.54
1:P:163:MET:HA	1:P:163:MET:HE2	1.89	0.54
3:P:673:BMA:O6	3:P:674:BMA:H62	2.07	0.54
1:P:151:ILE:HG23	1:P:469:ARG:HH12	1.71	0.54
1:P:280:PRO:HA	1:P:284:GLN:CD	2.27	0.54
1:P:380:GLU:HG2	1:P:466:TYR:CZ	2.42	0.54
1:P:241:GLN:HG2	1:P:245:ARG:CD	2.37	0.54
1:P:433:ARG:HH11	1:P:433:ARG:HG2	1.73	0.54
1:P:152:LEU:HB3	1:P:461:GLN:NE2	2.23	0.54
1:P:230:LEU:C	1:P:232:HIS:H	2.12	0.54
1:P:514:PRO:O	1:P:515:ASN:HB2	2.06	0.53
1:P:478:PHE:CE1	1:P:492:GLU:HA	2.43	0.53
1:P:51:GLY:N	1:P:54:ARG:HH21	2.06	0.53
1:P:150:ARG:NH1	1:P:154:SER:HA	2.23	0.53
1:P:191:PRO:CB	1:P:515:ASN:HA	2.36	0.53
1:P:517:ILE:HG23	1:P:518:PHE:CD1	2.43	0.53
1:P:49:ARG:HH11	1:P:49:ARG:HB3	1.73	0.53
1:P:246:LEU:CD1	1:P:253:LYS:HA	2.39	0.53
1:P:157:ARG:HA	1:P:459:ARG:HH11	1.74	0.53
1:P:574:THR:O	1:P:576:PRO:HD3	2.09	0.53
1:P:96:GLY:O	1:P:97:ARG:C	2.47	0.53
1:P:475:TYR:CD2	1:P:481:LEU:HA	2.44	0.53
1:P:287:VAL:HG21	1:P:292:PHE:HB2	1.91	0.52
1:P:279:ILE:O	1:P:281:PRO:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:518:PHE:CG	1:P:522:MET:HG2	2.45	0.52
1:P:408:LEU:HB3	1:P:409:PHE:CD1	2.43	0.52
1:P:234:TYR:OH	1:P:336:LEU:HD12	2.10	0.52
1:P:246:LEU:HD23	1:P:246:LEU:O	2.09	0.52
1:P:157:ARG:HA	1:P:459:ARG:NH1	2.25	0.52
1:P:306:LEU:C	1:P:306:LEU:HD23	2.30	0.52
1:P:255:GLN:NE2	1:P:265:SER:N	2.58	0.51
1:P:257:LEU:O	1:P:258:ASN:HB2	2.10	0.51
1:P:255:GLN:OE1	1:P:257:LEU:HD21	2.11	0.51
1:P:319:GLU:HB3	1:P:320:HIS:ND1	2.25	0.51
1:P:265:SER:HA	1:P:285:MET:HA	1.91	0.51
1:P:101:ASP:OD2	1:P:101:ASP:N	2.44	0.51
1:P:331:THR:O	1:P:335:ILE:HG13	2.11	0.51
1:P:373:TYR:CZ	1:P:541:SER:HA	2.46	0.51
1:P:295:LEU:HD12	1:P:295:LEU:N	2.26	0.51
1:P:338:GLY:HA3	1:P:559:VAL:HG13	1.93	0.50
1:P:582:VAL:CG2	1:P:583:PRO:HD2	2.37	0.50
1:P:348:TYR:HA	1:P:580:PHE:CD1	2.46	0.50
1:P:234:TYR:HE1	1:P:309:HIS:ND1	2.08	0.50
1:P:299:MET:HG3	1:P:414:LEU:CD2	2.42	0.50
1:P:247:PHE:N	1:P:247:PHE:CD1	2.80	0.50
1:P:88:PHE:CZ	1:P:92:LEU:HD11	2.47	0.50
1:P:389:PRO:HD3	1:P:440:ILE:HG12	1.94	0.50
1:P:501:LEU:HD21	1:P:506:GLY:HA2	1.92	0.50
1:P:210:PHE:CE1	1:P:382:ASN:HA	2.47	0.50
1:P:444:ILE:O	1:P:447:VAL:HG23	2.11	0.49
1:P:241:GLN:HE21	1:P:245:ARG:HD3	1.76	0.49
1:P:240:ARG:HE	1:P:288:GLY:HA2	1.77	0.49
1:P:171:LEU:CD1	1:P:456:ARG:HD3	2.42	0.49
1:P:263:PRO:HG2	1:P:299:MET:SD	2.53	0.49
1:P:60:THR:HG22	1:P:61:ARG:HG3	1.94	0.49
1:P:44:GLN:HG2	1:P:469:ARG:NE	2.28	0.49
1:P:296:PRO:HD2	1:P:407:PHE:CE2	2.47	0.49
1:P:178:SER:OG	1:P:449:VAL:HG22	2.12	0.49
1:P:408:LEU:HB3	1:P:409:PHE:CE1	2.47	0.49
1:P:475:TYR:CE2	1:P:481:LEU:HA	2.48	0.49
1:P:34:ASN:HB3	1:P:37:CYS:SG	2.53	0.49
1:P:323:TRP:CZ3	1:P:327:GLN:HG2	2.48	0.49
1:P:235:GLY:HA3	1:P:240:ARG:HD3	1.95	0.48
1:P:253:LYS:O	1:P:264:PRO:HD3	2.12	0.48
1:P:171:LEU:CB	1:P:456:ARG:NH1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:276:PRO:O	1:P:278:GLY:N	2.46	0.48
1:P:507:LEU:HD22	1:P:522:MET:SD	2.52	0.48
1:P:237:ASN:OD1	1:P:240:ARG:CB	2.61	0.48
1:P:246:LEU:HD13	1:P:253:LYS:HA	1.94	0.48
1:P:74:ILE:CG2	1:P:75:TRP:N	2.76	0.48
1:P:327:GLN:O	1:P:328:LEU:C	2.51	0.48
1:P:166:LYS:HD2	1:P:499:ASP:HB2	1.94	0.48
1:P:38:TYR:O	1:P:39:TYR:HB2	2.14	0.48
1:P:272:LEU:C	1:P:272:LEU:HD12	2.34	0.48
1:P:99:LEU:O	1:P:103:VAL:HG23	2.14	0.48
1:P:152:LEU:HD12	1:P:466:TYR:CE1	2.49	0.48
1:P:524:GLU:OE1	5:P:751:BOG:H2	2.14	0.48
1:P:74:ILE:HG23	1:P:75:TRP:N	2.28	0.48
1:P:204:HIS:HD2	1:P:232:HIS:HD2	1.59	0.47
1:P:298:LEU:H	1:P:298:LEU:HD12	1.77	0.47
1:P:280:PRO:HA	1:P:284:GLN:HG3	1.96	0.47
1:P:180:ARG:HA	1:P:180:ARG:NE	2.29	0.47
1:P:166:LYS:HD2	1:P:499:ASP:CB	2.45	0.47
1:P:120:ARG:NH1	1:P:120:ARG:HG3	2.29	0.47
1:P:137:ILE:H	1:P:137:ILE:CD1	2.25	0.47
1:P:120:ARG:HE	5:P:751:BOG:C6	2.28	0.47
1:P:261:VAL:HB	1:P:307:ARG:HD3	1.95	0.47
1:P:234:TYR:HE1	1:P:309:HIS:CE1	2.32	0.47
1:P:193:GLY:O	1:P:582:VAL:HG12	2.15	0.47
1:P:177:LEU:HD21	1:P:495:TYR:OH	2.15	0.47
1:P:478:PHE:CE2	1:P:491:LEU:HB3	2.49	0.47
1:P:374:ARG:HG2	1:P:374:ARG:O	2.14	0.47
1:P:301:TYR:HA	1:P:304:ILE:HD12	1.97	0.47
1:P:452:ILE:O	1:P:456:ARG:HG3	2.15	0.47
1:P:172:PRO:HG3	1:P:494:LEU:HB3	1.96	0.47
1:P:266:VAL:C	1:P:268:GLU:H	2.19	0.47
1:P:93:LEU:HD11	8:P:700:IM8:H222	1.96	0.46
1:P:262:TYR:HB3	1:P:285:MET:HE1	1.96	0.46
1:P:305:TRP:O	1:P:308:GLU:HB3	2.15	0.46
1:P:204:HIS:ND1	1:P:301:TYR:CB	2.78	0.46
1:P:254:TYR:CD2	1:P:254:TYR:N	2.82	0.46
1:P:280:PRO:N	1:P:281:PRO:CD	2.79	0.46
1:P:459:ARG:HH21	1:P:459:ARG:HG2	1.81	0.46
1:P:234:TYR:CE1	1:P:309:HIS:ND1	2.83	0.46
1:P:478:PHE:CD2	1:P:491:LEU:HB3	2.50	0.46
1:P:33:VAL:HG23	1:P:33:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:239:GLU:CD	1:P:239:GLU:N	2.68	0.46
1:P:209:PHE:HB2	1:P:377:ILE:HG13	1.96	0.46
1:P:391:MET:CG	7:P:601:HEM:HAB	2.38	0.45
1:P:320:HIS:O	1:P:323:TRP:HB2	2.15	0.45
1:P:255:GLN:HG2	1:P:264:PRO:HA	1.98	0.45
1:P:289:GLN:HB3	1:P:292:PHE:CD1	2.51	0.45
1:P:303:THR:HG22	1:P:307:ARG:HH21	1.80	0.45
1:P:306:LEU:O	1:P:306:LEU:HD23	2.15	0.45
1:P:291:VAL:HB	9:P:924:HOH:O	2.16	0.45
1:P:84:PRO:HB2	1:P:88:PHE:HD1	1.81	0.45
1:P:184:ARG:NH2	1:P:439:ASN:O	2.47	0.45
1:P:466:TYR:O	1:P:525:MET:HE2	2.16	0.45
1:P:495:TYR:HE2	1:P:502:GLU:HG3	1.82	0.45
1:P:527:ALA:N	1:P:528:PRO:CD	2.79	0.45
1:P:498:ILE:HG23	1:P:499:ASP:N	2.31	0.45
1:P:152:LEU:HD21	1:P:469:ARG:HB2	1.97	0.45
1:P:183:LEU:CD1	1:P:445:LEU:HD22	2.46	0.44
1:P:204:HIS:CE1	1:P:301:TYR:HB3	2.53	0.44
1:P:90:HIS:CE1	1:P:94:THR:HG21	2.53	0.44
1:P:243:GLN:CG	1:P:270:PRO:HG2	2.43	0.44
1:P:43:HIS:O	1:P:44:GLN:CB	2.66	0.44
1:P:348:TYR:HA	1:P:580:PHE:CE1	2.53	0.44
1:P:196:LEU:HA	1:P:196:LEU:HD23	1.83	0.44
1:P:88:PHE:O	1:P:92:LEU:HD13	2.18	0.44
3:P:673:BMA:C6	9:P:925:HOH:O	2.63	0.44
1:P:309:HIS:HB2	1:P:336:LEU:HD11	2.00	0.43
1:P:274:HIS:CD2	1:P:290:GLU:HB2	2.53	0.43
1:P:201:PHE:C	1:P:201:PHE:CD2	2.91	0.43
1:P:287:VAL:HG23	1:P:288:GLY:N	2.34	0.43
1:P:577:TYR:CZ	1:P:583:PRO:HB3	2.53	0.43
1:P:102:PHE:CE2	1:P:106:THR:HG21	2.54	0.43
1:P:34:ASN:HA	1:P:49:ARG:NH2	2.34	0.43
1:P:490:GLU:O	1:P:494:LEU:HG	2.19	0.43
1:P:501:LEU:HD12	1:P:502:GLU:H	1.83	0.43
1:P:442:HIS:HD2	1:P:443:HIS:H	1.66	0.43
1:P:344:VAL:CG1	1:P:534:LEU:HD11	2.49	0.43
1:P:241:GLN:HG2	1:P:245:ARG:HG3	1.99	0.43
1:P:204:HIS:HD2	1:P:232:HIS:CD2	2.30	0.43
1:P:418:GLY:O	1:P:419:VAL:C	2.57	0.43
1:P:239:GLU:O	1:P:242:TYR:N	2.52	0.43
1:P:409:PHE:O	1:P:411:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:383:GLN:HE22	1:P:455:SER:HB2	1.84	0.43
1:P:255:GLN:HE21	1:P:265:SER:N	2.17	0.42
1:P:195:ASN:O	1:P:198:PHE:HB3	2.18	0.42
1:P:149:THR:O	1:P:378:ALA:HA	2.19	0.42
1:P:233:ILE:O	1:P:288:GLY:HA3	2.19	0.42
1:P:566:LYS:HE2	1:P:566:LYS:HB3	1.84	0.42
1:P:275:TYR:CG	1:P:284:GLN:HG2	2.54	0.42
1:P:177:LEU:HD12	1:P:181:PHE:CD1	2.54	0.42
1:P:298:LEU:N	1:P:298:LEU:CD1	2.78	0.42
1:P:294:LEU:HB2	1:P:295:LEU:HD12	2.02	0.42
1:P:419:VAL:O	1:P:420:GLU:C	2.57	0.42
1:P:380:GLU:HG2	1:P:466:TYR:CE1	2.55	0.42
1:P:526:GLY:HA3	8:P:700:IM8:C12	2.49	0.42
1:P:521:SER:O	1:P:525:MET:HB2	2.19	0.42
1:P:563:THR:HG22	1:P:564:LEU:H	1.81	0.42
1:P:178:SER:CB	1:P:449:VAL:HG22	2.50	0.42
1:P:241:GLN:O	1:P:245:ARG:N	2.49	0.41
1:P:505:PRO:O	1:P:509:LEU:HG	2.20	0.41
1:P:204:HIS:NE2	1:P:232:HIS:CD2	2.89	0.41
1:P:556:PHE:CD1	1:P:560:LYS:HE3	2.55	0.41
1:P:384:LEU:C	1:P:384:LEU:HD23	2.41	0.41
1:P:564:LEU:HD13	1:P:578:VAL:CG2	2.51	0.41
1:P:563:THR:HB	1:P:566:LYS:HG3	2.01	0.41
1:P:388:HIS:N	1:P:389:PRO:CD	2.82	0.41
1:P:577:TYR:HE2	1:P:583:PRO:HD3	1.83	0.41
1:P:483:GLY:H	1:P:511:LYS:HB3	1.85	0.41
1:P:120:ARG:HG3	1:P:120:ARG:HH11	1.84	0.41
1:P:241:GLN:O	1:P:245:ARG:CG	2.65	0.41
1:P:179:ARG:O	1:P:183:LEU:HB3	2.21	0.41
1:P:254:TYR:HA	1:P:264:PRO:HD3	2.03	0.41
1:P:575:CYS:HA	1:P:576:PRO:HD2	1.95	0.41
1:P:345:ILE:HG22	1:P:346:GLU:N	2.35	0.41
1:P:254:TYR:CD1	1:P:261:VAL:HG13	2.57	0.40
1:P:240:ARG:HG3	1:P:271:VAL:CG2	2.26	0.40
1:P:303:THR:CG2	1:P:307:ARG:HH21	2.34	0.40
1:P:190:ASP:HA	1:P:191:PRO:HD2	1.94	0.40
1:P:253:LYS:CB	1:P:264:PRO:HG3	2.52	0.40
1:P:260:GLU:CB	1:P:262:TYR:CE1	3.02	0.40
1:P:34:ASN:OD1	1:P:36:CYS:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	551/600 (92%)	446 (81%)	81 (15%)	24 (4%)	3 10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	117	LEU
1	P	118	THR
1	P	158	ASP
1	P	247	PHE
1	P	277	ARG
1	P	281	PRO
1	P	469	ARG
1	P	328	LEU
1	P	545	TRP
1	P	551	GLY
1	P	327	GLN
1	P	96	GLY
1	P	97	ARG
1	P	204	HIS
1	P	226	HIS
1	P	268	GLU
1	P	270	PRO
1	P	392	PRO
1	P	468	LYS
1	P	484	GLU
1	P	267	GLU
1	P	280	PRO
1	P	290	GLU
1	P	33	VAL

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	P	458/530 (86%)	423 (92%)	35 (8%)	16 40

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	49	ARG
1	P	68	ASN
1	P	70	THR
1	P	74	ILE
1	P	101	ASP
1	P	111	THR
1	P	120	ARG
1	P	163	MET
1	P	180	ARG
1	P	185	ARG
1	P	209	PHE
1	P	272	LEU
1	P	284	GLN
1	P	289	GLN
1	P	290	GLU
1	P	291	VAL
1	P	322	THR
1	P	326	GLU
1	P	374	ARG
1	P	376	ARG
1	P	384	LEU
1	P	385	TYR
1	P	433	ARG
1	P	442	HIS
1	P	469	ARG
1	P	484	GLU
1	P	507	LEU
1	P	518	PHE
1	P	530	SER
1	P	554	VAL

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Mol	Chain	Res	Type
1	P	556	PHE
1	P	564	LEU
1	P	570	LEU
1	P	574	THR
1	P	579	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	42	GLN
1	P	43	HIS
1	P	56	GLN
1	P	90	HIS
1	P	192	GLN
1	P	203	GLN
1	P	208	GLN
1	P	241	GLN
1	P	274	HIS
1	P	330	GLN
1	P	358	GLN
1	P	375	ASN
1	P	383	GLN
1	P	443	HIS
1	P	557	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

8 carbohydrates 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	NAG	P	661	1,2	14,14,15	0.76	0	15,19,21	1.38	2 (13%)
2	NDG	P	662	2	14,14,15	0.74	0	15,19,21	0.91	1 (6%)
3	NAG	P	671	1,3	14,14,15	0.84	0	15,19,21	0.89	1 (6%)
3	NAG	P	672	3	14,14,15	1.06	0	15,19,21	1.20	1 (6%)
3	BMA	P	673	3	11,11,12	1.17	1 (9%)	14,15,17	1.72	3 (21%)
3	BMA	P	674	3	11,11,12	0.86	0	14,15,17	1.02	1 (7%)
4	NAG	P	681	1,4	14,14,15	0.67	0	15,19,21	0.82	1 (6%)
4	NAG	P	682	4	14,14,15	0.63	0	15,19,21	1.32	2 (13%)

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	NAG	P	661	1,2	-	0/6/23/26	0/1/1/1
2	NDG	P	662	2	-	0/6/23/26	0/1/1/1
3	NAG	P	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	672	3	-	0/6/23/26	0/1/1/1
3	BMA	P	673	3	-	0/2/19/22	0/1/1/1
3	BMA	P	674	3	-	0/2/19/22	1/1/1/1
4	NAG	P	681	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	682	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	673	BMA	C1-C2	2.44	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	682	NAG	C2-N2-C7	-3.59	118.43	123.04
3	P	672	NAG	C4-C3-C2	-3.56	105.70	111.23
2	P	661	NAG	C4-C3-C2	-2.97	106.61	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	661	NAG	C2-N2-C7	-2.90	119.31	123.04
4	P	682	NAG	C4-C3-C2	-2.68	107.06	111.23
4	P	681	NAG	C2-N2-C7	-2.46	119.88	123.04
3	P	671	NAG	C2-N2-C7	-2.22	120.18	123.04
2	P	662	NDG	C3-C4-C5	2.07	113.81	110.20
3	P	673	BMA	O5-C1-C2	2.14	114.32	110.86
3	P	673	BMA	C1-O5-C5	2.47	115.39	112.25
3	P	674	BMA	C1-O5-C5	3.15	116.25	112.25
3	P	673	BMA	C1-C2-C3	5.30	115.81	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	674	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	672	NAG	1	0
3	P	673	BMA	3	0
3	P	674	BMA	1	0

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
7	HEM	P	601	1	30,50,50	2.40	8 (26%)	24,82,82	2.79	10 (41%)
8	IM8	P	700	-	29,32,32	1.79	9 (31%)	34,45,45	1.90	8 (23%)
5	BOG	P	750	-	12,12,20	0.88	1 (8%)	17,17,25	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BOG	P	751	-	12,12,20	1.11	1 (8%)	17,17,25	0.90	0
6	FLC	P	900	-	3,12,12	0.29	0	3,17,17	0.61	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
7	HEM	P	601	1	-	0/10/54/54	0/0/8/8
8	IM8	P	700	-	-	0/18/22/22	0/3/3/3
5	BOG	P	750	-	-	0/2/22/31	0/1/1/1
5	BOG	P	751	-	-	0/2/22/31	0/1/1/1
6	FLC	P	900	-	-	0/6/16/16	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	601	HEM	C2D-C3D	-6.38	1.35	1.54
7	P	601	HEM	C3D-C4D	-5.50	1.44	1.51
7	P	601	HEM	C3B-C4B	-4.12	1.48	1.51
7	P	601	HEM	C2C-C1C	-3.58	1.45	1.52
7	P	601	HEM	C3C-CAC	-3.19	1.45	1.51
8	P	700	IM8	C17-C18	-2.95	1.44	1.51
8	P	700	IM8	C15-C14	2.01	1.42	1.38
5	P	750	BOG	C1-C2	2.10	1.56	1.52
8	P	700	IM8	C14-C13	2.14	1.42	1.38
7	P	601	HEM	FE-NC	2.21	2.04	1.95
8	P	700	IM8	C12-C11	2.24	1.42	1.38
8	P	700	IM8	O-C3	2.25	1.42	1.37
7	P	601	HEM	CBC-CAC	2.34	1.42	1.29
5	P	751	BOG	C4-C5	2.45	1.58	1.53
8	P	700	IM8	C12-C13	2.91	1.43	1.38
8	P	700	IM8	C15-C10	3.18	1.44	1.39
8	P	700	IM8	C2-C3	3.92	1.44	1.37
8	P	700	IM8	C4-C3	4.02	1.46	1.38
7	P	601	HEM	CAA-C2A	4.76	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	700	IM8	C3-C2-C1	-2.80	115.76	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	700	IM8	C16-C8-C7	-2.68	123.16	129.08
7	P	601	HEM	CAA-C2A-C3A	-2.54	121.74	129.00
8	P	700	IM8	O-C3-C2	-2.43	118.51	124.62
8	P	700	IM8	C16-C8-N	2.02	125.02	122.44
8	P	700	IM8	C19-N2-C18	2.82	126.95	122.79
7	P	601	HEM	CAD-C3D-C4D	3.38	124.39	112.47
7	P	601	HEM	C3C-CAC-CBC	3.40	129.67	124.46
7	P	601	HEM	CBA-CAA-C2A	3.48	118.76	112.53
8	P	700	IM8	C2-C1-C	3.81	124.21	119.65
7	P	601	HEM	C2D-C3D-C4D	4.23	108.67	101.50
7	P	601	HEM	CMD-C2D-C3D	4.36	133.64	114.35
8	P	700	IM8	C10-C9-N	4.64	123.99	118.02
7	P	601	HEM	CAD-C3D-C2D	4.77	126.93	113.22
7	P	601	HEM	CMC-C2C-C3C	4.77	128.45	116.53
7	P	601	HEM	CMB-C2B-C3B	4.78	128.46	116.53
7	P	601	HEM	CAA-C2A-C1A	4.83	132.25	127.01
8	P	700	IM8	C7-C1-C	5.51	113.34	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	601	HEM	6	0
8	P	700	IM8	5	0
5	P	751	BOG	5	0
6	P	900	FLC	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, 95^{th} 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	P	553/600 (92%)	-0.17	6 (1%) 82 80	35, 61, 87, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	483	GLY	4.0
1	P	256	MET	2.9
1	P	258	ASN	2.5
1	P	368	GLY	2.3
1	P	488	ALA	2.2
1	P	503	PHE	2.1

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

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

6.3 Carbohydrates

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, 95^{th} 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(Å^2)	Q<0.9
2	NAG	P	661	14/15	0.93	0.27	1.85	78,78,78,78	0
3	NAG	P	671	14/15	0.90	0.13	-0.79	61,61,61,61	0
4	NAG	P	681	14/15	0.96	0.12	-1.08	77,77,77,77	0
3	NAG	P	672	14/15	0.89	0.27	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BMA	P	673	11/12	0.88	0.29	-	89,89,89,89	0
3	BMA	P	674	11/12	0.56	0.32	-	77,77,77,77	11
4	NAG	P	682	14/15	0.88	0.27	-	92,92,92,92	0
2	NDG	P	662	14/15	0.89	0.39	-	87,87,87,87	0

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, 95^{th} 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(Å^2)	Q<0.9
5	BOG	P	751	12/20	0.81	0.29	2.89	61,61,61,61	0
8	IM8	P	700	30/30	0.90	0.23	0.91	81,81,81,81	0
6	FLC	P	900	13/13	0.83	0.22	0.89	67,67,67,67	13
7	HEM	P	601	43/43	0.93	0.21	0.01	73,73,73,73	0
5	BOG	P	750	12/20	0.85	0.50	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.