Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:23 PM GMT

PDB ID	:	1FE2
Title	:	CRYSTAL STRUCTURE OF DIHOMO-GAMMA-LINOLEIC ACID BOUND IN THE CYCLOOXYGENASE CHANNEL OF PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE-1.
Authors	:	Thuresson, E.D.; Malkowski, M.G.; Lakkides, K.M.; Smith, W.L.; Garavito, R.M.
Deposited on	:	2000-07-20
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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 (i)) were used in the production of this report:

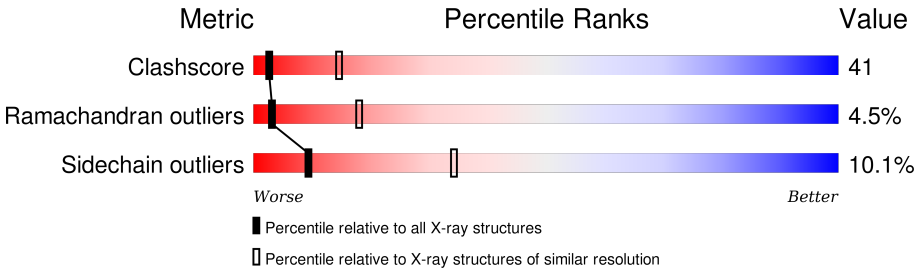
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	39% 48% 9% •

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	NAG	A	662	X	-	-	-
3	BMA	A	675	X	-	-	-
4	BOG	A	751	-	-	X	-
6	LAX	A	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4699 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 ENDOPEROXIDE H SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4397	2855	734	780	28			

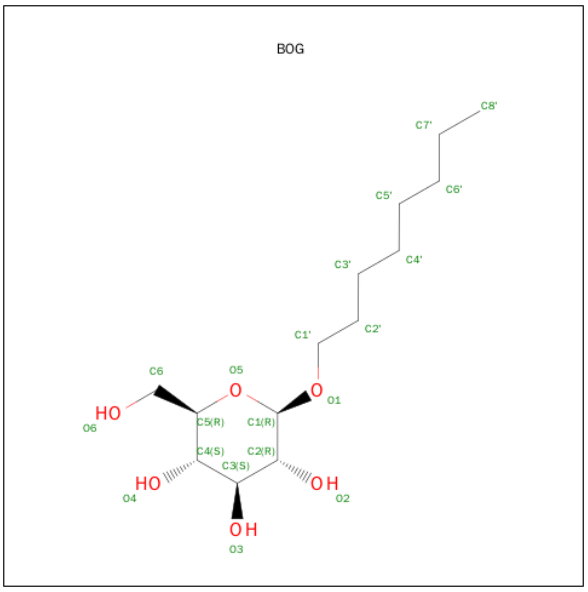
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

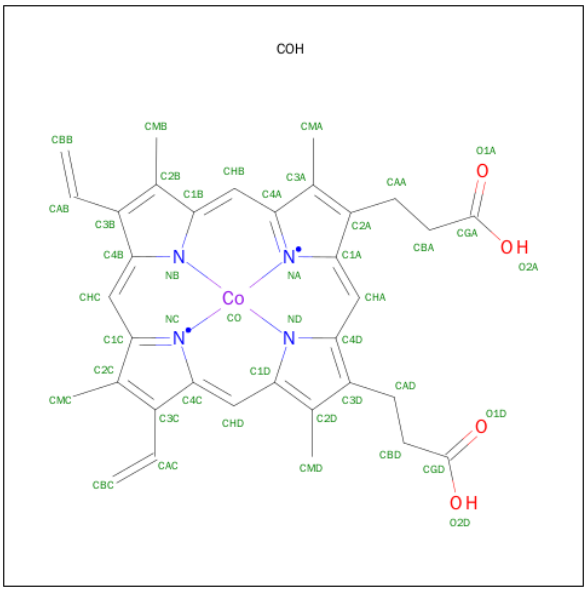
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



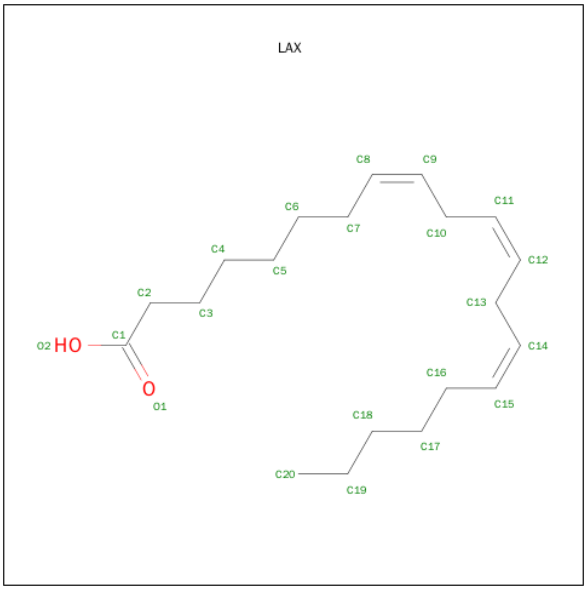
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	A	1	Total C O 20 14 6	0	0
4	A	1	Total C O 20 14 6	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is EICOSA-8,11,14-TRIENOIC ACID (three-letter code: LAX) (formula: $C_{20}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	20	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		

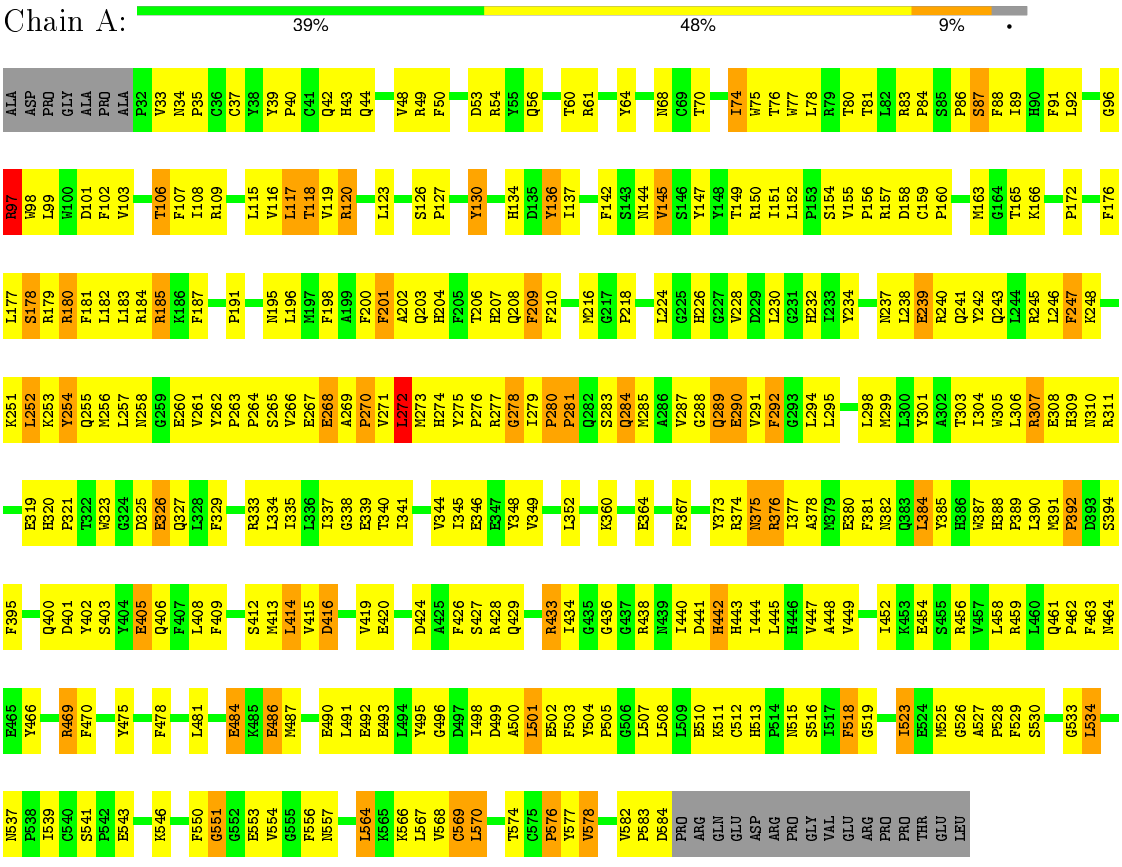
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: PROSTAGLANDIN ENDOPEROXIDE H SYNTHASE-1

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	182.19Å 182.19Å 103.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.4 (20.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4699	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COH, BMA, LAX, NAG, 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	A	0.45	0/4536	0.70	0/6179

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
2	A	1	0
3	A	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	662	NAG	C1
3	A	675	BMA	C1

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	4397	0	4203	360	0
2	A	56	0	50	5	0
3	A	61	0	52	3	0
4	A	60	0	84	16	0
5	A	43	0	30	2	0
6	A	22	0	33	22	0
7	A	60	0	0	7	0
All	All	4699	0	4452	370	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 41.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:661:NAG:H61	2:A:662:NAG:H82	1.35	1.08
1:A:97:ARG:HH21	1:A:97:ARG:HB2	1.18	1.04
1:A:98:TRP:HB2	4:A:752:BOG:H5'1	1.46	0.95
1:A:251:LYS:HB3	1:A:310:ASN:ND2	1.84	0.93
1:A:97:ARG:NH2	1:A:97:ARG:HB2	1.83	0.92
1:A:243:GLN:HG3	1:A:270:PRO:HG2	1.49	0.92
1:A:294:LEU:O	1:A:295:LEU:HG	1.70	0.90
1:A:239:GLU:CD	1:A:239:GLU:H	1.75	0.89
1:A:501:LEU:HD12	1:A:502:GLU:H	1.38	0.89
1:A:530:SER:OG	6:A:700:LAX:H132	1.76	0.85
1:A:195:ASN:ND2	1:A:427:SER:HA	1.92	0.84
1:A:344:VAL:O	1:A:348:TYR:HB3	1.77	0.84
1:A:272:LEU:HD12	1:A:273:MET:H	1.45	0.80
1:A:87:SER:HB2	4:A:750:BOG:H62	1.63	0.79
1:A:523:ILE:HG23	6:A:700:LAX:H62	1.63	0.79
1:A:533:GLY:HA3	6:A:700:LAX:H203	1.65	0.78
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.65	0.78
1:A:89:ILE:HG23	4:A:751:BOG:H8'1	1.66	0.78
1:A:208:GLN:NE2	1:A:230:LEU:H	1.84	0.76
1:A:513:HIS:HB2	1:A:516:SER:OG	1.85	0.76
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.68	0.75
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.66	0.75
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.67	0.74
1:A:326:GLU:OE1	1:A:326:GLU:HA	1.88	0.74
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.68	0.74
1:A:543:GLU:O	1:A:546:LYS:HE3	1.87	0.74
1:A:120:ARG:NE	4:A:751:BOG:H1	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:CD2	1:A:247:PHE:HZ	2.06	0.73
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.70	0.73
1:A:501:LEU:HD12	1:A:502:GLU:N	2.02	0.73
1:A:137:ILE:H	1:A:137:ILE:HD12	1.52	0.73
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.29	0.73
1:A:120:ARG:CZ	4:A:751:BOG:H1	2.18	0.72
1:A:442:HIS:CD2	1:A:443:HIS:H	2.08	0.72
1:A:89:ILE:HG23	4:A:751:BOG:C8'	2.20	0.72
1:A:391:MET:HG3	5:A:601:COH:HAB	1.72	0.71
1:A:462:PRO:HB3	1:A:499:ASP:O	1.91	0.70
1:A:272:LEU:HD12	1:A:273:MET:N	2.06	0.70
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.71	0.70
1:A:263:PRO:HD2	1:A:285:MET:CE	2.20	0.70
1:A:115:LEU:HD23	4:A:751:BOG:H5'2	1.72	0.70
1:A:60:THR:HG22	1:A:61:ARG:HG3	1.74	0.69
1:A:526:GLY:C	6:A:700:LAX:H9	2.13	0.69
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.28	0.69
1:A:384:LEU:HD23	1:A:384:LEU:C	2.12	0.69
1:A:237:ASN:ND2	1:A:240:ARG:H	1.91	0.68
1:A:130:TYR:HB3	1:A:134:HIS:O	1.92	0.68
1:A:334:LEU:HD23	1:A:337:ILE:HD12	1.75	0.67
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.29	0.67
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.10	0.67
1:A:150:ARG:NH1	1:A:154:SER:HB3	2.10	0.67
1:A:172:PRO:HB2	1:A:177:LEU:HD13	1.76	0.67
1:A:512:CYS:HA	1:A:519:GLY:HA2	1.75	0.66
1:A:137:ILE:N	1:A:137:ILE:HD12	2.10	0.66
1:A:352:LEU:HD23	6:A:700:LAX:H71	1.78	0.66
1:A:253:LYS:O	1:A:254:TYR:HB3	1.96	0.66
1:A:344:VAL:O	1:A:349:VAL:HG23	1.96	0.65
1:A:172:PRO:CB	1:A:177:LEU:HD13	2.25	0.65
1:A:412:SER:O	1:A:416:ASP:HB2	1.96	0.65
1:A:178:SER:OG	1:A:449:VAL:HG22	1.96	0.65
1:A:89:ILE:HD12	4:A:751:BOG:H8'3	1.78	0.65
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.97	0.65
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.78	0.65
6:A:700:LAX:C8	6:A:700:LAX:H41	2.27	0.65
1:A:334:LEU:HA	1:A:337:ILE:HD12	1.78	0.65
1:A:442:HIS:HD2	1:A:443:HIS:H	1.44	0.64
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.79	0.64
1:A:279:ILE:HG22	1:A:279:ILE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG22	7:A:852:HOH:O	1.97	0.64
1:A:495:TYR:OH	1:A:502:GLU:HG3	1.98	0.64
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.61	0.64
1:A:102:PHE:O	1:A:106:THR:HG23	1.98	0.63
1:A:126:SER:HA	1:A:127:PRO:C	2.19	0.63
1:A:530:SER:OG	6:A:700:LAX:H101	1.98	0.63
1:A:258:ASN:HD21	1:A:415:VAL:HG12	1.62	0.63
1:A:414:LEU:HD12	1:A:414:LEU:O	1.99	0.63
1:A:39:TYR:OH	1:A:155:VAL:HG22	1.99	0.63
1:A:463:PHE:HB2	1:A:502:GLU:O	1.98	0.63
1:A:226:HIS:HB3	1:A:377:ILE:HG12	1.81	0.63
1:A:287:VAL:HG23	1:A:289:GLN:H	1.64	0.62
1:A:202:ALA:O	1:A:206:THR:HG23	1.98	0.62
1:A:442:HIS:CD2	1:A:443:HIS:N	2.66	0.62
2:A:661:NAG:H61	2:A:662:NAG:C8	2.22	0.62
1:A:388:HIS:HB3	1:A:444:ILE:CD1	2.28	0.62
1:A:88:PHE:O	1:A:91:PHE:HB3	1.99	0.62
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.34	0.62
1:A:258:ASN:ND2	1:A:415:VAL:HG12	2.15	0.62
1:A:263:PRO:HD2	1:A:285:MET:HE1	1.81	0.61
1:A:40:PRO:HB3	2:A:661:NAG:H62	1.82	0.61
1:A:207:HIS:HB3	1:A:289:GLN:HE21	1.65	0.61
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.36	0.61
1:A:237:ASN:HB2	1:A:239:GLU:OE1	2.01	0.61
1:A:444:ILE:O	1:A:447:VAL:HG23	2.00	0.61
1:A:424:ASP:O	1:A:428:ARG:HD2	2.01	0.61
1:A:255:GLN:HE21	1:A:264:PRO:HA	1.65	0.60
1:A:265:SER:HA	1:A:285:MET:HA	1.82	0.60
1:A:564:LEU:HD22	1:A:578:VAL:CG2	2.32	0.60
1:A:352:LEU:HD23	6:A:700:LAX:C7	2.31	0.60
1:A:97:ARG:O	1:A:101:ASP:OD2	2.19	0.60
1:A:582:VAL:HG22	1:A:583:PRO:O	2.02	0.60
1:A:463:PHE:HE1	1:A:507:LEU:HG	1.66	0.60
1:A:179:ARG:HA	1:A:183:LEU:HB2	1.84	0.60
1:A:412:SER:O	1:A:416:ASP:N	2.31	0.59
1:A:196:LEU:HD11	1:A:429:GLN:NE2	2.16	0.59
1:A:109:ARG:NH2	1:A:360:LYS:HB2	2.18	0.59
1:A:120:ARG:HD2	4:A:751:BOG:O2	2.02	0.59
1:A:257:LEU:O	1:A:258:ASN:HB2	2.01	0.59
1:A:204:HIS:CD2	1:A:232:HIS:CD2	2.91	0.59
1:A:182:LEU:HB3	1:A:440:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:NH2	1:A:325:ASP:OD2	2.36	0.59
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.38	0.58
1:A:263:PRO:HD2	1:A:285:MET:HE2	1.84	0.58
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.38	0.58
1:A:243:GLN:HG3	1:A:270:PRO:CG	2.29	0.58
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.39	0.58
1:A:279:ILE:C	1:A:281:PRO:CD	2.72	0.58
1:A:237:ASN:HD21	1:A:240:ARG:HB2	1.69	0.58
1:A:86:PRO:HA	4:A:751:BOG:H62	1.84	0.58
1:A:163:MET:HE2	1:A:163:MET:HA	1.85	0.58
1:A:566:LYS:O	1:A:570:LEU:HB2	2.04	0.58
1:A:96:GLY:O	1:A:98:TRP:N	2.36	0.57
1:A:292:PHE:CD1	1:A:298:LEU:HD23	2.40	0.57
1:A:185:ARG:HD2	1:A:185:ARG:N	2.18	0.57
1:A:337:ILE:O	1:A:341:ILE:HG13	2.04	0.57
1:A:246:LEU:O	1:A:246:LEU:HG	2.04	0.57
1:A:216:MET:HG2	3:A:672:NAG:C8	2.33	0.57
1:A:230:LEU:C	1:A:232:HIS:H	2.07	0.57
1:A:77:TRP:O	1:A:81:THR:HG23	2.04	0.57
1:A:333:ARG:O	1:A:337:ILE:HG13	2.05	0.57
1:A:185:ARG:NH1	1:A:438:ARG:NH1	2.53	0.57
1:A:319:GLU:HB3	1:A:320:HIS:ND1	2.20	0.57
1:A:523:ILE:CG2	6:A:700:LAX:H62	2.34	0.56
1:A:279:ILE:N	1:A:280:PRO:HD3	2.20	0.56
1:A:280:PRO:N	1:A:281:PRO:HD3	2.19	0.56
1:A:415:VAL:HG23	7:A:857:HOH:O	2.05	0.56
1:A:243:GLN:CG	1:A:270:PRO:HG2	2.31	0.56
1:A:204:HIS:CD2	1:A:232:HIS:HD2	2.23	0.56
1:A:115:LEU:O	1:A:119:VAL:HG23	2.05	0.55
1:A:403:SER:N	1:A:406:GLN:OE1	2.38	0.55
1:A:484:GLU:OE2	1:A:487:MET:N	2.39	0.55
1:A:216:MET:HG2	3:A:672:NAG:H82	1.88	0.55
1:A:388:HIS:N	1:A:389:PRO:HD2	2.22	0.55
1:A:109:ARG:HH21	1:A:360:LYS:HB2	1.71	0.55
1:A:242:TYR:CD2	1:A:247:PHE:CZ	2.93	0.55
1:A:254:TYR:CD1	1:A:261:VAL:HG13	2.41	0.54
1:A:340:THR:O	1:A:344:VAL:HG23	2.08	0.54
1:A:87:SER:CB	4:A:750:BOG:H62	2.33	0.54
1:A:149:THR:O	1:A:378:ALA:HA	2.05	0.54
1:A:335:ILE:O	1:A:339:GLU:HG3	2.07	0.54
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD22	1:A:578:VAL:HG21	1.88	0.54
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.88	0.54
1:A:151:ILE:HG23	1:A:469:ARG:NH1	2.23	0.54
1:A:391:MET:HA	1:A:391:MET:CE	2.37	0.54
1:A:254:TYR:HD1	1:A:261:VAL:HG13	1.73	0.53
1:A:414:LEU:HD12	1:A:414:LEU:C	2.28	0.53
1:A:452:ILE:O	1:A:456:ARG:HG3	2.08	0.53
1:A:470:PHE:CD1	1:A:525:MET:HA	2.43	0.53
1:A:152:LEU:HD12	1:A:466:TYR:CE1	2.43	0.53
1:A:245:ARG:HB2	1:A:247:PHE:CE1	2.43	0.53
1:A:513:HIS:CE1	1:A:523:ILE:HD11	2.43	0.53
1:A:238:LEU:O	1:A:241:GLN:HB3	2.08	0.53
1:A:308:GLU:O	1:A:311:ARG:HB3	2.09	0.53
1:A:408:LEU:HB3	1:A:409:PHE:CE1	2.44	0.53
1:A:134:HIS:HB3	1:A:136:TYR:CE1	2.44	0.53
1:A:320:HIS:O	1:A:323:TRP:HB2	2.08	0.53
1:A:298:LEU:N	1:A:298:LEU:HD12	2.24	0.53
1:A:40:PRO:O	1:A:68:ASN:HB3	2.08	0.53
1:A:181:PHE:O	1:A:438:ARG:N	2.42	0.53
1:A:226:HIS:HB3	1:A:377:ILE:H	1.74	0.52
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.44	0.52
1:A:195:ASN:HD22	1:A:427:SER:HA	1.73	0.52
1:A:201:PHE:C	1:A:201:PHE:CD2	2.81	0.52
1:A:142:PHE:O	1:A:376:ARG:NH2	2.43	0.52
1:A:408:LEU:HB3	1:A:409:PHE:CD1	2.44	0.52
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.45	0.52
1:A:258:ASN:ND2	1:A:415:VAL:CG1	2.73	0.52
1:A:201:PHE:HD2	1:A:201:PHE:C	2.12	0.52
1:A:348:TYR:CE2	6:A:700:LAX:H14	2.46	0.52
1:A:384:LEU:HD23	1:A:384:LEU:O	2.10	0.52
1:A:295:LEU:HD21	1:A:408:LEU:HD23	1.92	0.51
1:A:537:ASN:OD1	1:A:539:ILE:HG23	2.11	0.51
1:A:380:GLU:HG2	1:A:466:TYR:CZ	2.46	0.51
1:A:261:VAL:HB	1:A:307:ARG:HD2	1.93	0.51
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.41	0.51
1:A:163:MET:HA	1:A:163:MET:CE	2.40	0.51
1:A:530:SER:OG	6:A:700:LAX:H161	2.11	0.51
1:A:201:PHE:HD2	1:A:201:PHE:O	1.94	0.51
4:A:752:BOG:C4'	4:A:752:BOG:H8'2	2.40	0.51
1:A:513:HIS:HB2	1:A:516:SER:CB	2.41	0.51
1:A:413:MET:HE3	7:A:856:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HB3	1:A:454:GLU:HG3	1.92	0.51
1:A:89:ILE:CD1	4:A:751:BOG:H8'3	2.41	0.51
1:A:403:SER:OG	1:A:405:GLU:HG2	2.11	0.51
4:A:752:BOG:H4'1	4:A:752:BOG:H8'2	1.93	0.51
1:A:306:LEU:HD23	1:A:306:LEU:C	2.32	0.50
1:A:530:SER:O	1:A:534:LEU:HD22	2.11	0.50
1:A:278:GLY:C	1:A:280:PRO:HD3	2.32	0.50
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.47	0.50
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.75	0.50
1:A:413:MET:HA	2:A:681:NAG:O6	2.11	0.50
1:A:75:TRP:CE3	1:A:78:LEU:HD12	2.46	0.50
1:A:238:LEU:HB3	1:A:239:GLU:OE2	2.11	0.50
1:A:568:VAL:HG12	1:A:569:CYS:N	2.25	0.50
1:A:518:PHE:HZ	6:A:700:LAX:H72	1.76	0.50
1:A:228:VAL:O	1:A:337:ILE:HG23	2.12	0.49
1:A:201:PHE:HB2	1:A:301:TYR:CZ	2.47	0.49
1:A:137:ILE:CD1	1:A:137:ILE:H	2.21	0.49
1:A:157:ARG:NH1	1:A:459:ARG:HD2	2.26	0.49
1:A:204:HIS:ND1	1:A:301:TYR:CB	2.76	0.49
1:A:120:ARG:NH1	6:A:700:LAX:O2	2.45	0.49
1:A:289:GLN:HB3	1:A:292:PHE:CD1	2.47	0.49
1:A:43:HIS:O	1:A:44:GLN:HB2	2.12	0.49
1:A:287:VAL:HG23	1:A:288:GLY:N	2.27	0.49
1:A:478:PHE:CE1	1:A:498:ILE:HA	2.48	0.49
1:A:498:ILE:HG23	1:A:499:ASP:N	2.26	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.95	0.48
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.49	0.48
1:A:373:TYR:CZ	1:A:541:SER:HA	2.48	0.48
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.95	0.48
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.39	0.48
1:A:266:VAL:HG21	1:A:284:GLN:HE22	1.78	0.48
1:A:392:PRO:HG3	1:A:429:GLN:NE2	2.29	0.48
1:A:149:THR:HG22	1:A:377:ILE:O	2.13	0.48
1:A:200:PHE:O	1:A:203:GLN:N	2.47	0.48
1:A:257:LEU:O	1:A:258:ASN:CB	2.61	0.48
3:A:673:BMA:O6	3:A:674:BMA:H62	2.13	0.48
1:A:145:VAL:HG13	1:A:226:HIS:HE2	1.78	0.47
1:A:458:LEU:O	1:A:459:ARG:HB2	2.13	0.47
1:A:384:LEU:C	1:A:384:LEU:CD2	2.82	0.47
1:A:490:GLU:O	1:A:493:GLU:HB3	2.14	0.47
1:A:241:GLN:O	1:A:245:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:CG2	1:A:75:TRP:N	2.77	0.47
6:A:700:LAX:C11	6:A:700:LAX:H71	2.44	0.47
1:A:419:VAL:O	1:A:420:GLU:C	2.52	0.47
1:A:478:PHE:CE2	1:A:491:LEU:HB3	2.50	0.47
1:A:448:ALA:O	1:A:452:ILE:HG13	2.14	0.47
1:A:305:TRP:O	1:A:308:GLU:HB3	2.15	0.47
1:A:433:ARG:NH1	1:A:436:GLY:HA3	2.29	0.47
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.28	0.47
1:A:272:LEU:O	1:A:273:MET:HG2	2.13	0.47
1:A:527:ALA:N	6:A:700:LAX:H9	2.29	0.47
1:A:208:GLN:HE22	1:A:230:LEU:H	1.61	0.47
1:A:151:ILE:CG2	1:A:469:ARG:NH1	2.78	0.47
1:A:103:VAL:HG13	1:A:108:ILE:CG2	2.45	0.47
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.50	0.47
1:A:200:PHE:O	1:A:201:PHE:C	2.54	0.47
1:A:333:ARG:HG2	1:A:337:ILE:HD11	1.97	0.47
1:A:523:ILE:HA	6:A:700:LAX:H8	1.96	0.46
1:A:239:GLU:CD	1:A:239:GLU:N	2.56	0.46
1:A:88:PHE:CE2	1:A:92:LEU:HD11	2.50	0.46
1:A:441:ASP:OD2	1:A:442:HIS:HD2	1.97	0.46
1:A:267:GLU:O	1:A:268:GLU:HB2	2.14	0.46
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.50	0.46
1:A:204:HIS:ND1	1:A:301:TYR:HB2	2.30	0.46
1:A:461:GLN:HB3	1:A:462:PRO:CD	2.45	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.50	0.46
1:A:42:GLN:NE2	7:A:827:HOH:O	2.49	0.46
1:A:74:ILE:HG22	1:A:75:TRP:N	2.30	0.45
1:A:239:GLU:OE2	1:A:239:GLU:N	2.48	0.45
1:A:345:ILE:HG22	1:A:346:GLU:N	2.30	0.45
1:A:183:LEU:HB2	1:A:445:LEU:HD22	1.97	0.45
1:A:490:GLU:HG3	7:A:835:HOH:O	2.15	0.45
1:A:237:ASN:OD1	1:A:240:ARG:HB3	2.17	0.45
1:A:245:ARG:HD2	1:A:329:PHE:CE2	2.52	0.45
1:A:253:LYS:O	1:A:254:TYR:CB	2.63	0.45
1:A:274:HIS:CD2	1:A:290:GLU:HB2	2.52	0.45
1:A:309:HIS:CD2	1:A:309:HIS:C	2.89	0.45
1:A:145:VAL:HG11	1:A:224:LEU:HB3	1.98	0.45
1:A:246:LEU:HD12	1:A:253:LYS:HG2	1.98	0.45
1:A:181:PHE:HZ	1:A:490:GLU:HG2	1.82	0.45
1:A:117:LEU:O	1:A:118:THR:C	2.54	0.45
1:A:269:ALA:O	1:A:271:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ALA:O	1:A:501:LEU:C	2.56	0.44
1:A:280:PRO:N	1:A:281:PRO:CD	2.80	0.44
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.53	0.44
1:A:208:GLN:HG2	1:A:209:PHE:CD1	2.52	0.44
1:A:107:PHE:CD2	1:A:107:PHE:N	2.85	0.44
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.53	0.44
1:A:34:ASN:HB2	1:A:158:ASP:OD2	2.17	0.44
1:A:116:VAL:O	1:A:120:ARG:HB2	2.17	0.44
1:A:523:ILE:HG22	6:A:700:LAX:C3	2.47	0.44
1:A:200:PHE:HE2	1:A:426:PHE:CE1	2.35	0.44
1:A:338:GLY:O	1:A:339:GLU:C	2.55	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.53	0.44
1:A:191:PRO:HG2	1:A:515:ASN:O	2.17	0.44
1:A:381:PHE:HB2	1:A:529:PHE:CG	2.52	0.44
1:A:442:HIS:HE2	1:A:443:HIS:CE1	2.34	0.44
1:A:134:HIS:HB3	1:A:136:TYR:CD1	2.52	0.44
1:A:512:CYS:HA	1:A:519:GLY:CA	2.45	0.44
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.52	0.44
1:A:252:LEU:HD11	1:A:329:PHE:HE1	1.83	0.44
1:A:84:PRO:HB2	1:A:88:PHE:HD1	1.83	0.44
1:A:144:ASN:HB3	1:A:147:TYR:HD2	1.82	0.44
1:A:292:PHE:O	1:A:299:MET:HE2	2.18	0.43
1:A:486:GLU:O	1:A:487:MET:C	2.56	0.43
1:A:123:LEU:O	1:A:469:ARG:NH2	2.50	0.43
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.82	0.43
1:A:349:VAL:CG1	6:A:700:LAX:H51	2.48	0.43
1:A:103:VAL:HG13	1:A:108:ILE:HG22	2.00	0.43
1:A:276:PRO:HA	7:A:842:HOH:O	2.18	0.43
1:A:201:PHE:CD2	1:A:201:PHE:O	2.71	0.43
1:A:256:MET:SD	1:A:261:VAL:HG22	2.59	0.43
1:A:107:PHE:C	1:A:109:ARG:N	2.71	0.43
1:A:96:GLY:C	1:A:98:TRP:H	2.21	0.43
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.59	0.43
1:A:106:THR:OG1	1:A:108:ILE:HG13	2.18	0.43
1:A:550:PHE:O	1:A:551:GLY:O	2.36	0.43
1:A:204:HIS:ND1	1:A:301:TYR:HB3	2.34	0.43
1:A:176:PHE:O	1:A:180:ARG:HB2	2.19	0.43
1:A:87:SER:HB2	4:A:750:BOG:C6	2.42	0.43
1:A:96:GLY:C	1:A:98:TRP:N	2.72	0.43
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.54	0.43
1:A:185:ARG:HD3	1:A:438:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:C	1:A:323:TRP:H	2.22	0.42
1:A:64:TYR:CZ	1:A:76:THR:HG21	2.54	0.42
1:A:237:ASN:HD21	1:A:240:ARG:H	1.65	0.42
1:A:294:LEU:HD22	1:A:409:PHE:HD2	1.76	0.42
6:A:700:LAX:C4	6:A:700:LAX:C8	2.96	0.42
1:A:246:LEU:O	1:A:248:LYS:N	2.52	0.42
1:A:553:GLU:O	1:A:557:ASN:ND2	2.52	0.42
1:A:523:ILE:H	1:A:523:ILE:HG13	1.56	0.42
1:A:208:GLN:HB3	1:A:232:HIS:CG	2.54	0.42
1:A:230:LEU:HA	1:A:232:HIS:ND1	2.34	0.42
1:A:461:GLN:HB3	1:A:462:PRO:HD2	2.02	0.42
1:A:145:VAL:HG13	1:A:226:HIS:NE2	2.34	0.42
1:A:502:GLU:HB2	1:A:505:PRO:HD2	2.01	0.42
1:A:179:ARG:O	1:A:183:LEU:HB3	2.20	0.42
1:A:568:VAL:O	1:A:570:LEU:N	2.53	0.42
1:A:394:SER:C	1:A:395:PHE:CD1	2.93	0.42
1:A:352:LEU:CD2	6:A:700:LAX:H11	2.50	0.42
1:A:75:TRP:O	1:A:78:LEU:N	2.52	0.42
1:A:510:GLU:HG2	1:A:511:LYS:O	2.20	0.42
1:A:271:VAL:HG22	1:A:272:LEU:N	2.35	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.77	0.42
1:A:527:ALA:HB2	6:A:700:LAX:C4	2.50	0.41
1:A:390:LEU:HD21	1:A:434:ILE:HD11	2.02	0.41
1:A:86:PRO:HA	4:A:751:BOG:C6	2.50	0.41
1:A:178:SER:HB3	1:A:445:LEU:HD11	2.02	0.41
1:A:266:VAL:CG2	1:A:284:GLN:NE2	2.83	0.41
1:A:290:GLU:H	1:A:290:GLU:CD	2.21	0.41
1:A:464:ASN:OD1	1:A:475:TYR:N	2.52	0.41
1:A:492:GLU:O	1:A:496:GLY:N	2.44	0.41
1:A:107:PHE:HD2	1:A:107:PHE:H	1.65	0.41
1:A:295:LEU:HD11	5:A:601:COH:HBB1	2.03	0.41
1:A:304:ILE:CG2	1:A:567:LEU:HG	2.51	0.41
1:A:184:ARG:NH1	1:A:187:PHE:HD2	2.19	0.41
1:A:179:ARG:HA	1:A:183:LEU:CB	2.49	0.41
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.97	0.41
1:A:266:VAL:CG2	1:A:284:GLN:HE22	2.33	0.41
1:A:53:ASP:OD2	1:A:54:ARG:HG3	2.20	0.41
1:A:375:ASN:HD22	1:A:375:ASN:HA	1.71	0.41
1:A:251:LYS:HD3	1:A:310:ASN:HD22	1.85	0.41
1:A:500:ALA:O	1:A:501:LEU:O	2.39	0.41
1:A:442:HIS:NE2	1:A:443:HIS:CE1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:C	1:A:281:PRO:HD3	2.41	0.40
1:A:299:MET:HG3	1:A:414:LEU:HD23	2.03	0.40
1:A:275:TYR:CG	1:A:284:GLN:HG2	2.55	0.40
1:A:289:GLN:HB3	1:A:292:PHE:CG	2.56	0.40
1:A:196:LEU:HD21	1:A:392:PRO:HD3	2.03	0.40
1:A:255:GLN:NE2	1:A:265:SER:N	2.68	0.40
1:A:303:THR:O	1:A:307:ARG:HB2	2.22	0.40
1:A:279:ILE:N	1:A:280:PRO:CD	2.85	0.40
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.48	0.40
2:A:682:NAG:H2	7:A:850:HOH:O	2.21	0.40
6:A:700:LAX:H101	6:A:700:LAX:H132	1.79	0.40
1:A:35:PRO:C	1:A:37:CYS:H	2.25	0.40
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.03	0.40
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.53	0.40
1:A:50:PHE:CE2	1:A:56:GLN:NE2	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	551/576 (96%)	430 (78%)	96 (17%)	25 (4%)	3 18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	247	PHE
1	A	281	PRO
1	A	97	ARG
1	A	178	SER
1	A	268	GLU

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	292	PHE
1	A	501	LEU
1	A	551	GLY
1	A	569	CYS
1	A	272	LEU
1	A	278	GLY
1	A	486	GLU
1	A	254	TYR
1	A	118	THR
1	A	160	PRO
1	A	400	GLN
1	A	401	ASP
1	A	576	PRO
1	A	280	PRO
1	A	392	PRO
1	A	481	LEU
1	A	145	VAL
1	A	270	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	466/506 (92%)	419 (90%)	47 (10%)	9 34

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	49	ARG
1	A	70	THR
1	A	74	ILE
1	A	80	THR
1	A	87	SER
1	A	97	ARG

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	106	THR
1	A	120	ARG
1	A	130	TYR
1	A	136	TYR
1	A	180	ARG
1	A	185	ARG
1	A	201	PHE
1	A	209	PHE
1	A	239	GLU
1	A	252	LEU
1	A	272	LEU
1	A	283	SER
1	A	284	GLN
1	A	289	GLN
1	A	290	GLU
1	A	307	ARG
1	A	326	GLU
1	A	374	ARG
1	A	375	ASN
1	A	376	ARG
1	A	384	LEU
1	A	385	TYR
1	A	405	GLU
1	A	414	LEU
1	A	416	ASP
1	A	433	ARG
1	A	442	HIS
1	A	469	ARG
1	A	484	GLU
1	A	518	PHE
1	A	523	ILE
1	A	534	LEU
1	A	554	VAL
1	A	556	PHE
1	A	564	LEU
1	A	570	LEU
1	A	574	THR
1	A	578	VAL
1	A	584	ASP

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

Mol	Chain	Res	Type
1	A	42	GLN
1	A	43	HIS
1	A	56	GLN
1	A	203	GLN
1	A	208	GLN
1	A	232	HIS
1	A	241	GLN
1	A	255	GLN
1	A	258	ASN
1	A	274	HIS
1	A	284	GLN
1	A	310	ASN
1	A	375	ASN
1	A	443	HIS
1	A	557	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 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	A	661	1,2	14,14,15	0.66	0	15,19,21	1.27	2 (13%)
2	NAG	A	662	2	14,14,15	0.83	0	15,19,21	1.15	1 (6%)
3	NAG	A	671	1,3	14,14,15	0.60	0	15,19,21	0.87	0
3	NAG	A	672	3	14,14,15	1.12	1 (7%)	15,19,21	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	A	673	3	11,11,12	1.15	1 (9%)	14,15,17	1.34	2 (14%)
3	BMA	A	674	3	11,11,12	1.19	1 (9%)	14,15,17	1.22	2 (14%)
3	BMA	A	675	3	11,11,12	0.88	0	14,15,17	0.86	1 (7%)
2	NAG	A	681	1,2	14,14,15	0.64	0	15,19,21	0.70	0
2	NAG	A	682	2	14,14,15	0.71	0	15,19,21	1.18	1 (6%)

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	A	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	662	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	BMA	A	673	3	-	0/2/19/22	0/1/1/1
3	BMA	A	674	3	-	0/2/19/22	1/1/1/1
3	BMA	A	675	3	1/1/4/5	0/2/19/22	1/1/1/1
2	NAG	A	681	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	682	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	674	BMA	C1-C2	2.03	1.57	1.52
3	A	673	BMA	C1-C2	2.23	1.57	1.52
3	A	672	NAG	O4-C4	2.28	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	682	NAG	C2-N2-C7	-3.48	118.57	123.04
2	A	661	NAG	C4-C3-C2	-3.40	105.95	111.23
3	A	672	NAG	C4-C3-C2	-3.36	106.01	111.23
2	A	661	NAG	C2-N2-C7	-2.18	120.24	123.04
3	A	675	BMA	C1-O5-C5	2.26	115.12	112.25
3	A	674	BMA	O3-C3-C2	2.36	114.26	110.00
3	A	673	BMA	C1-O5-C5	2.42	115.33	112.25
2	A	662	NAG	C4-C3-C2	2.73	115.47	111.23
3	A	674	BMA	C1-O5-C5	3.24	116.36	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	673	BMA	C1-C2-C3	3.95	114.22	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	662	NAG	C1
3	A	675	BMA	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	675	BMA	C1-C2-C3-C4-C5-O5
3	A	674	BMA	C1-C2-C3-C4-C5-O5

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	3	0
2	A	662	NAG	2	0
3	A	672	NAG	2	0
3	A	673	BMA	1	0
3	A	674	BMA	1	0
2	A	681	NAG	1	0
2	A	682	NAG	1	0

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	COH	A	601	1	28,50,50	1.70	7 (25%)	19,82,82	2.41	9 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	LAX	A	700	-	18,21,21	0.61	0	18,21,21	1.04	1 (5%)
4	BOG	A	750	-	20,20,20	0.54	0	25,25,25	0.60	1 (4%)
4	BOG	A	751	-	20,20,20	0.48	0	25,25,25	0.99	2 (8%)
4	BOG	A	752	-	20,20,20	0.67	0	25,25,25	0.77	1 (4%)

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
5	COH	A	601	1	-	0/6/54/54	0/0/8/8
6	LAX	A	700	-	-	0/17/19/19	0/0/0/0
4	BOG	A	750	-	-	0/11/31/31	0/1/1/1
4	BOG	A	751	-	-	0/11/31/31	0/1/1/1
4	BOG	A	752	-	-	0/11/31/31	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COH	C3B-C2B	-2.56	1.36	1.40
5	A	601	COH	CBC-CAC	2.22	1.44	1.28
5	A	601	COH	C2A-C3A	2.41	1.44	1.37
5	A	601	COH	CMC-C2C	2.58	1.57	1.51
5	A	601	COH	CAD-C3D	2.73	1.56	1.52
5	A	601	COH	C4D-ND	3.06	1.44	1.36
5	A	601	COH	CAA-C2A	4.84	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	COH	CAD-C3D-C4D	-4.19	122.46	127.01
6	A	700	LAX	C14-C13-C12	2.03	118.74	112.00
5	A	601	COH	CAD-CBD-CGD	2.19	116.76	112.75
4	A	750	BOG	O1-C1-C2	2.21	110.83	108.04
5	A	601	COH	CMA-C3A-C2A	2.24	129.91	125.24
4	A	752	BOG	O1-C1-C2	2.36	111.02	108.04
5	A	601	COH	CAA-CBA-CGA	2.39	117.13	112.75
4	A	751	BOG	O1-C1-C2	2.72	111.48	108.04
5	A	601	COH	CAA-C2A-C1A	2.90	130.16	127.01
5	A	601	COH	CBA-CAA-C2A	2.92	117.76	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	751	BOG	C1'-O1-C1	3.11	119.39	113.94
5	A	601	COH	C2A-C1A-NA	3.13	111.50	108.70
5	A	601	COH	C3D-C4D-ND	4.14	112.45	108.74
5	A	601	COH	CMD-C2D-C3D	4.15	133.91	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	COH	2	0
6	A	700	LAX	22	0
4	A	750	BOG	3	0
4	A	751	BOG	10	0
4	A	752	BOG	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.