Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:52 PM GMT

PDB ID	:	1CVU
Title	:	CRYSTAL STRUCTURE OF ARACHIDONIC ACID BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2
Authors	:	Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on	:	1999-08-24
Resolution	:	2.40 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:

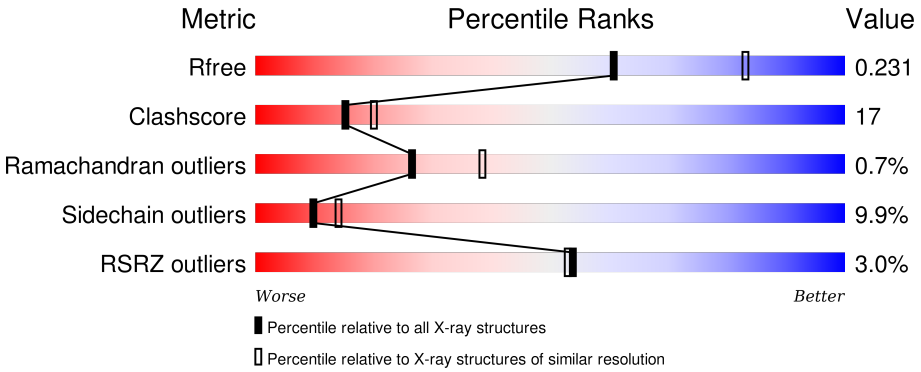
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	A	552	2% 68% 25% 7%
1	B	552	3% 66% 27% 7%
2	F	9	56% 44% 44% 11%

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
3	NAG	A	661	-	-	-	X
3	NAG	B	2661	-	-	-	X
4	NAG	A	672	-	-	-	X
4	MAN	A	674	X	-	-	-
4	MAN	B	2674	X	-	-	-
5	NAG	A	681	-	-	-	X
5	NAG	B	2681	-	-	-	X
6	BOG	A	702	-	-	-	X
6	BOG	A	704	-	-	-	X
6	BOG	B	2702	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 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 H2 SYNTHASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4469	2883	746	815	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	ENGINEERED	UNP Q05769
A	333	LYS	ARG	ENGINEERED	UNP Q05769
B	2310	GLN	ASN	ENGINEERED	UNP Q05769
B	2333	LYS	ARG	ENGINEERED	UNP Q05769

- Molecule 2 is a protein called PROTEIN (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	9	Total	C	N	O	0	0	0
			63	37	11	15			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

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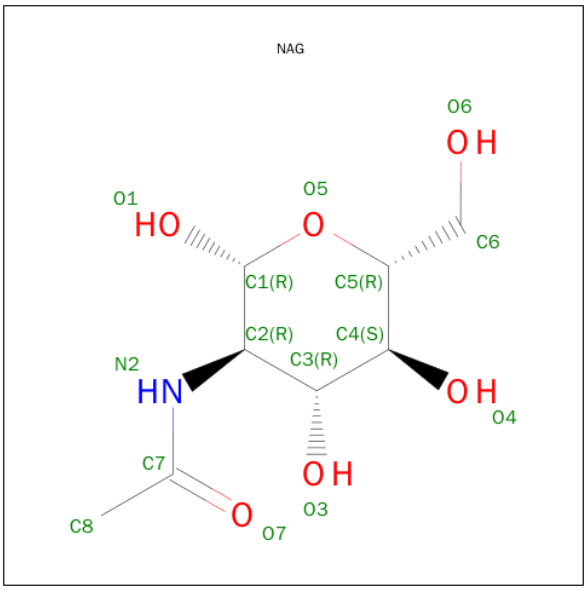
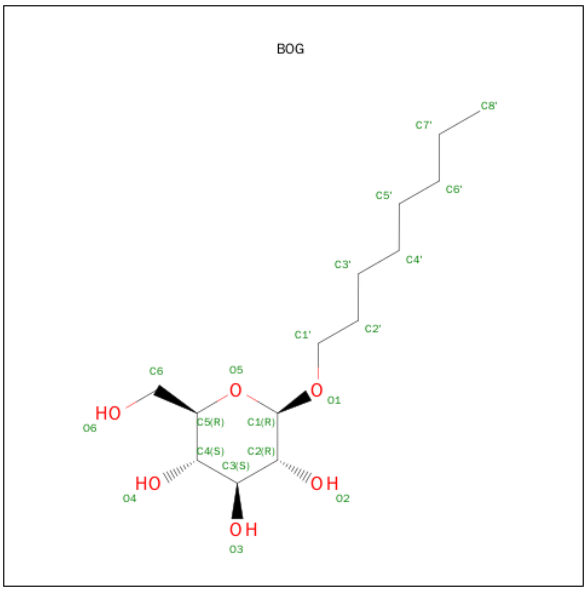
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



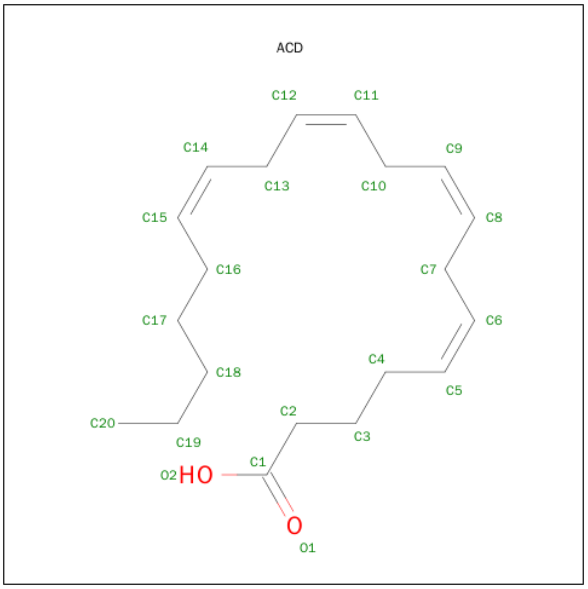
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 7 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$).



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

- Molecule 8 is water.

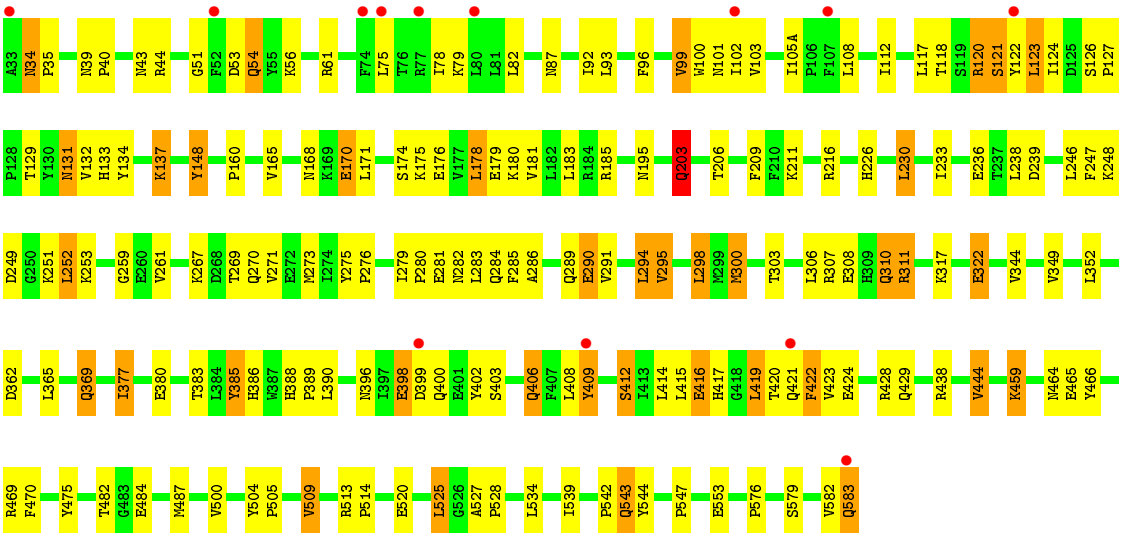
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	410	Total O 410 410	0	0
8	B	361	Total O 361 361	0	0

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.

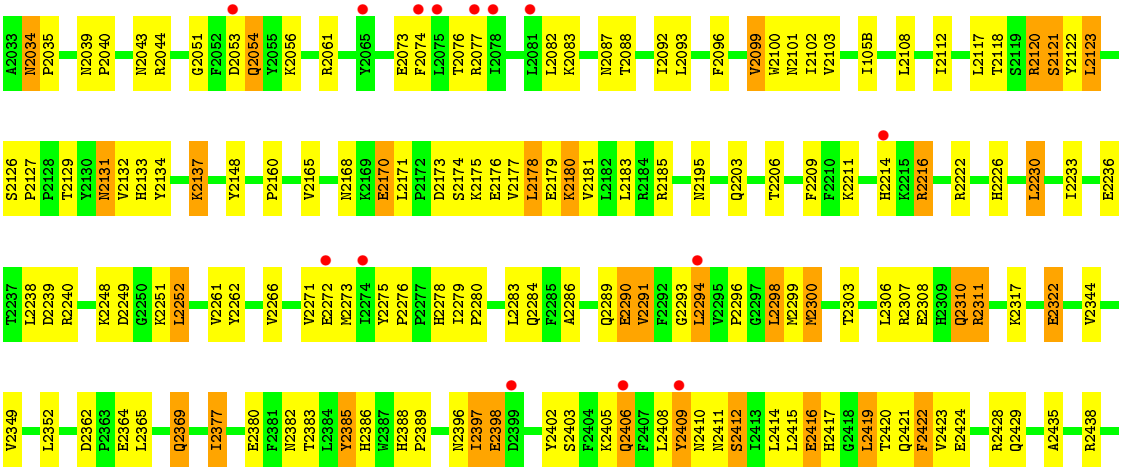
• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-2

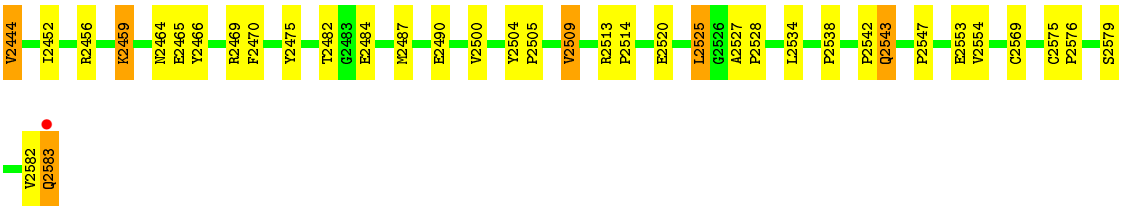
Chain A:



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-2

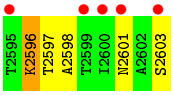
Chain B:





- Molecule 2: PROTEIN (9-MER)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.04Å 133.96Å 124.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 34.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (35.00-2.40) 96.2 (34.95-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.235 0.204 , 0.231	Depositor DCC
R_{free} test set	3887 reflections (6.80%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 57179 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: ACD, BOG, NAG, MAN

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	0.49	3/4595 (0.1%)	0.65	1/6229 (0.0%)
1	B	0.49	2/4595 (0.0%)	0.68	2/6229 (0.0%)
2	F	1.87	2/62 (3.2%)	1.70	2/82 (2.4%)
All	All	0.51	7/9252 (0.1%)	0.68	5/12540 (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	A	0	1
4	A	1	0
4	B	1	0
All	All	2	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2603	SER	C-O	9.63	1.41	1.23
2	F	2603	SER	C-OXT	-7.12	1.09	1.23
1	A	203	GLN	CD-OE1	5.84	1.36	1.24
1	B	2170	GLU	CD-OE2	5.66	1.31	1.25
1	B	2170	GLU	CD-OE1	5.66	1.31	1.25
1	A	170	GLU	CD-OE1	5.62	1.31	1.25
1	A	170	GLU	CD-OE2	5.38	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2603	SER	CA-C-O	11.83	144.95	120.10
1	B	2216	ARG	NE-CZ-NH1	-9.59	115.50	120.30
2	F	2603	SER	N-CA-C	6.91	129.66	111.00
1	B	2216	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	148	TYR	N-CA-C	-5.18	97.01	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	674	MAN	C1
4	B	2674	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4469	0	4373	154	0
1	B	4469	0	4373	163	0
2	F	63	0	65	8	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	50	0	42	3	0
4	B	50	0	42	5	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	60	0	84	6	0
6	B	40	0	56	6	0
7	A	22	0	31	0	0
7	B	22	0	31	0	0
8	A	410	0	0	8	0
8	B	361	0	0	11	0
All	All	10100	0	9173	321	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 17.

All (321) 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:2251:LYS:HD3	1:B:2310:GLN:HG3	1.49	0.92
1:A:251:LYS:HD3	1:A:310:GLN:HG3	1.51	0.89
1:B:2408:LEU:O	1:B:2409:TYR:HB2	1.74	0.87
1:B:2283:LEU:HD21	1:B:2415:LEU:HD12	1.55	0.85
1:A:543:GLN:HA	1:A:543:GLN:OE1	1.77	0.85
1:B:2209:PHE:HB2	1:B:2377:ILE:HD13	1.59	0.83
1:B:2543:GLN:OE1	1:B:2543:GLN:HA	1.77	0.83
1:A:209:PHE:HB2	1:A:377:ILE:HD13	1.60	0.81
1:A:246:LEU:HG	1:A:248:LYS:HG3	1.64	0.79
1:B:2216:ARG:NH1	4:B:2672:NAG:C7	2.47	0.78
1:A:300:MET:HE3	1:A:422:PHE:HB3	1.66	0.76
1:A:75:LEU:HD11	1:A:79:LYS:HE3	1.68	0.76
1:B:2275:TYR:HB3	1:B:2279:ILE:HD13	1.68	0.76
1:B:2300:MET:HE3	1:B:2422:PHE:HB3	1.66	0.76
2:F:2597:THR:HG22	2:F:2601:ASN:HD22	1.52	0.75
1:B:2464:ASN:HD21	1:B:2475:TYR:H	1.36	0.74
2:F:2597:THR:CG2	2:F:2601:ASN:ND2	2.51	0.73
1:A:51:GLY:C	1:B:2322:GLU:HG2	2.10	0.72
1:B:2209:PHE:HB2	1:B:2377:ILE:CD1	2.19	0.71
1:A:464:ASN:HD21	1:A:475:TYR:H	1.37	0.71
2:F:2597:THR:HG23	2:F:2601:ASN:HD21	1.54	0.70
1:A:322:GLU:HG2	1:B:2051:GLY:C	2.11	0.70
1:A:129:THR:HG22	1:A:137:LYS:HD3	1.72	0.70
1:B:2582:VAL:HG13	1:B:2583:GLN:OE1	1.91	0.70
2:F:2597:THR:HG23	2:F:2601:ASN:ND2	2.07	0.69
1:A:209:PHE:HB2	1:A:377:ILE:CD1	2.22	0.69
1:B:2129:THR:HG22	1:B:2137:LYS:HD3	1.76	0.68
1:A:582:VAL:HG13	1:A:583:GLN:OE1	1.92	0.68
1:A:412:SER:O	1:A:416:GLU:HB2	1.94	0.67
1:A:396:ASN:H	1:A:429:GLN:HE22	1.44	0.66
1:A:424:GLU:O	1:A:428:ARG:HG3	1.96	0.66
1:B:2276:PRO:O	1:B:2279:ILE:HD12	1.95	0.65
1:A:300:MET:CE	1:A:422:PHE:HB3	2.26	0.65
1:B:2061:ARG:HD2	8:B:3380:HOH:O	1.96	0.65
1:B:2131:ASN:C	1:B:2131:ASN:HD22	2.00	0.65
1:B:2300:MET:CE	1:B:2422:PHE:HB3	2.26	0.65
1:B:2271:VAL:HG21	1:B:2286:ALA:HB1	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HH11	6:A:703:BOG:H4'1	1.61	0.64
1:A:469:ARG:O	1:A:469:ARG:HD2	1.98	0.64
1:A:131:ASN:C	1:A:131:ASN:HD22	2.00	0.63
1:B:2414:LEU:HD11	1:B:2419:LEU:HD22	1.81	0.63
1:A:398:GLU:OE1	1:A:417:HIS:HD2	1.81	0.63
1:A:75:LEU:HD12	1:A:75:LEU:O	1.99	0.63
1:B:2293:GLY:HA2	1:B:2299:MET:CE	2.29	0.63
1:B:2283:LEU:HD21	1:B:2415:LEU:CD1	2.26	0.62
1:B:2527:ALA:HB3	1:B:2528:PRO:HD3	1.82	0.62
1:B:2424:GLU:O	1:B:2428:ARG:HG3	1.99	0.62
1:B:2216:ARG:HG2	4:B:2672:NAG:O7	1.98	0.62
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.82	0.62
1:A:543:GLN:HB2	8:A:3119:HOH:O	1.99	0.62
2:F:2597:THR:HG22	2:F:2601:ASN:ND2	2.14	0.61
1:B:2211:LYS:NZ	1:B:2236:GLU:HG2	2.15	0.61
1:A:251:LYS:CD	1:A:310:GLN:HG3	2.30	0.61
1:A:185:ARG:NH1	6:A:703:BOG:H4'1	2.16	0.61
1:A:444:VAL:HG13	1:A:444:VAL:O	1.99	0.61
1:A:273:MET:SD	1:A:290:GLU:HA	2.40	0.60
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.81	0.60
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.84	0.60
1:A:211:LYS:NZ	1:A:236:GLU:HG2	2.17	0.59
1:B:2203:GLN:HG2	1:B:2298:LEU:HD11	1.83	0.59
1:A:420:THR:HG23	1:A:576:PRO:HG3	1.84	0.59
1:B:2398:GLU:OE2	1:B:2421:GLN:HG2	2.02	0.59
1:B:2293:GLY:HA2	1:B:2299:MET:HE3	1.83	0.59
1:B:2251:LYS:CD	1:B:2310:GLN:HG3	2.29	0.59
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.85	0.59
1:B:2293:GLY:O	1:B:2411:ASN:ND2	2.30	0.58
1:B:2230:LEU:HD13	1:B:2233:ILE:HD12	1.84	0.58
1:B:2402:TYR:OH	1:B:2417:HIS:HE1	1.86	0.58
1:B:2053:ASP:C	1:B:2054:GLN:HG3	2.23	0.58
1:B:2280:PRO:HG2	1:B:2283:LEU:HD12	1.85	0.58
1:B:2482:THR:HG22	1:B:2509:VAL:HG13	1.86	0.58
1:A:203:GLN:OE1	6:A:704:BOG:H5'1	2.04	0.58
1:A:294:LEU:HA	1:A:409:TYR:CE2	2.37	0.58
1:B:2469:ARG:HD2	1:B:2469:ARG:O	2.03	0.58
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.69	0.58
1:B:2181:VAL:HG12	1:B:2487:MET:HG2	1.87	0.57
1:A:53:ASP:C	1:A:54:GLN:HG3	2.25	0.57
1:B:2108:LEU:O	1:B:2112:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105(B):ILE:HG22	1:B:2108:LEU:H	1.68	0.57
4:A:672:NAG:H61	4:A:673:MAN:C1	2.35	0.57
1:B:2310:GLN:HG2	8:B:3241:HOH:O	2.04	0.56
1:B:2148:TYR:HD1	1:B:2377:ILE:HG22	1.70	0.56
1:B:2364:GLU:HG3	8:B:3734:HOH:O	2.05	0.56
1:B:2383:THR:HA	1:B:2386:HIS:CD2	2.41	0.56
1:A:280:PRO:O	1:A:284:GLN:HG3	2.04	0.56
1:A:543:GLN:O	1:B:2137:LYS:HE2	2.07	0.55
1:A:108:LEU:O	1:A:112:ILE:HG12	2.06	0.55
1:B:2444:VAL:O	1:B:2444:VAL:HG13	2.06	0.55
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.41	0.55
1:A:137:LYS:HE2	1:B:2543:GLN:O	2.06	0.55
1:B:2211:LYS:NZ	1:B:2236:GLU:CG	2.69	0.55
1:A:195:ASN:HB3	1:A:582:VAL:HG23	1.89	0.55
1:B:2120:ARG:HG2	1:B:2120:ARG:HH11	1.71	0.55
4:B:2672:NAG:H61	4:B:2673:MAN:C1	2.37	0.55
1:B:2500:VAL:HG12	1:B:2500:VAL:O	2.07	0.55
1:B:2396:ASN:H	1:B:2429:GLN:HE22	1.55	0.54
1:B:2470:PHE:CG	1:B:2525:LEU:HD22	2.42	0.54
1:B:2420:THR:HG23	1:B:2576:PRO:HG3	1.89	0.54
1:B:2412:SER:O	1:B:2416:GLU:HB2	2.06	0.54
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.71	0.54
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.43	0.53
2:F:2596:LYS:HD2	2:F:2597:THR:H	1.73	0.53
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.70	0.53
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.39	0.53
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.91	0.53
1:B:2575:CYS:SG	2:F:2598:ALA:HA	2.49	0.53
1:B:2148:TYR:CD1	1:B:2377:ILE:HG22	2.43	0.53
1:B:2203:GLN:OE1	6:B:2704:BOG:H5'1	2.09	0.53
1:B:2403:SER:OG	1:B:2406:GLN:HG3	2.09	0.53
1:A:226:HIS:C	1:A:377:ILE:HD12	2.30	0.52
1:B:2195:ASN:HB3	1:B:2582:VAL:HG23	1.90	0.52
1:B:2271:VAL:O	1:B:2271:VAL:HG23	2.08	0.52
1:B:2226:HIS:C	1:B:2377:ILE:HD12	2.30	0.52
1:B:2175:LYS:O	1:B:2179:GLU:HG3	2.10	0.52
1:A:75:LEU:CD1	1:A:79:LYS:HG3	2.40	0.51
1:B:2276:PRO:HD2	1:B:2279:ILE:CD1	2.39	0.51
1:B:2582:VAL:O	1:B:2582:VAL:HG12	2.11	0.51
1:A:175:LYS:O	1:A:179:GLU:HG3	2.11	0.51
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:O	1:A:270:GLN:HB2	2.10	0.51
1:B:2296:PRO:HG3	1:B:2410:ASN:O	2.10	0.51
1:B:2083:LYS:HE2	8:B:3296:HOH:O	2.10	0.51
1:A:465:GLU:HA	1:A:465:GLU:OE1	2.10	0.51
1:B:2504:TYR:HB3	1:B:2505:PRO:HD3	1.92	0.51
1:B:2276:PRO:HB2	1:B:2278:HIS:CE1	2.46	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.94	0.50
1:B:2240:ARG:NH2	1:B:2273:MET:CE	2.74	0.50
1:B:2102:ILE:HG13	1:B:2103:VAL:N	2.27	0.50
1:A:261:VAL:O	1:A:307:ARG:NH1	2.44	0.50
1:A:513:ARG:NH2	1:A:520:GLU:HG3	2.27	0.50
1:A:383:THR:HA	1:A:386:HIS:CD2	2.47	0.50
1:A:280:PRO:HB2	1:A:282:ASN:OD1	2.11	0.50
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.95	0.50
1:B:2039:ASN:N	1:B:2040:PRO:CD	2.75	0.49
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.93	0.49
1:A:267:LYS:HD3	1:A:281:GLU:OE1	2.11	0.49
1:A:582:VAL:O	1:A:582:VAL:HG12	2.12	0.49
1:B:2034:ASN:C	1:B:2034:ASN:HD22	2.16	0.49
1:A:206:THR:HG21	1:A:385:TYR:CE2	2.48	0.49
1:B:2291:VAL:O	1:B:2294:LEU:HG	2.13	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.93	0.49
1:B:2131:ASN:HD21	1:B:2134:TYR:HD1	1.61	0.49
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.48	0.49
1:A:179:GLU:OE2	6:A:703:BOG:H1	2.13	0.48
1:A:403:SER:OG	1:A:406:GLN:HG2	2.13	0.48
1:B:2121:SER:O	1:B:2123:LEU:N	2.46	0.48
1:A:121:SER:O	1:A:123:LEU:N	2.46	0.48
1:B:2294:LEU:N	1:B:2294:LEU:HD23	2.27	0.48
1:A:131:ASN:HD21	1:A:134:TYR:HD1	1.60	0.48
1:A:500:VAL:HG12	1:A:500:VAL:O	2.14	0.48
1:A:132:VAL:HG13	1:A:133:HIS:CD2	2.49	0.48
1:A:39:ASN:N	1:A:40:PRO:CD	2.77	0.48
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.13	0.48
1:A:102:ILE:HG13	1:A:103:VAL:N	2.26	0.48
1:B:2414:LEU:HA	1:B:2422:PHE:CE1	2.49	0.48
1:B:2174:SER:O	1:B:2178:LEU:HB2	2.13	0.48
1:B:2099:VAL:O	1:B:2102:ILE:HG12	2.14	0.47
1:A:421:GLN:HG2	8:A:3103:HOH:O	2.15	0.47
1:A:131:ASN:ND2	1:A:134:TYR:H	2.12	0.47
1:B:2102:ILE:CG1	1:B:2103:VAL:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2275:TYR:O	1:B:2276:PRO:C	2.52	0.47
1:A:99:VAL:O	1:A:102:ILE:HG12	2.14	0.47
1:B:2126:SER:HA	1:B:2127:PRO:C	2.34	0.47
1:B:2465:GLU:HA	1:B:2465:GLU:OE1	2.14	0.47
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.48	0.47
1:A:174:SER:O	1:A:178:LEU:HB2	2.14	0.47
1:A:273:MET:HG3	1:A:285:PHE:O	2.14	0.47
1:A:294:LEU:HD23	1:A:295:VAL:HG23	1.97	0.47
1:A:295:VAL:CG2	1:A:298:LEU:HD22	2.44	0.47
1:A:34:ASN:C	1:A:34:ASN:HD22	2.17	0.47
1:A:43:ASN:O	1:A:44:ARG:HB2	2.15	0.47
1:A:547:PRO:HB3	1:A:553:GLU:OE1	2.14	0.47
1:B:2513:ARG:NH2	1:B:2520:GLU:HG3	2.30	0.47
1:B:2176:GLU:O	1:B:2180:LYS:HG3	2.15	0.46
1:B:2249:ASP:OD2	1:B:2317:LYS:HE2	2.15	0.46
1:B:2569:CYS:SG	2:F:2597:THR:HG22	2.55	0.46
1:A:303:THR:O	1:A:307:ARG:HD3	2.16	0.46
1:A:102:ILE:CG1	1:A:103:VAL:N	2.78	0.46
1:B:2262:TYR:CZ	1:B:2415:LEU:HD23	2.50	0.46
1:B:2386:HIS:CE1	6:B:2704:BOG:H1'2	2.51	0.46
1:A:126:SER:HA	1:A:127:PRO:C	2.36	0.46
1:A:176:GLU:O	1:A:180:LYS:HG3	2.16	0.46
1:B:2380:GLU:HG2	1:B:2466:TYR:CE1	2.51	0.46
1:B:2132:VAL:HG13	1:B:2133:HIS:CD2	2.51	0.46
1:B:2397:ILE:HD12	1:B:2422:PHE:CZ	2.51	0.46
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.29	0.46
1:A:226:HIS:HA	1:A:377:ILE:HD12	1.98	0.46
1:B:2419:LEU:O	1:B:2423:VAL:HG23	2.15	0.45
1:B:2290:GLU:H	1:B:2290:GLU:HG3	1.39	0.45
1:A:252:LEU:O	1:A:310:GLN:NE2	2.49	0.45
1:B:105(B):ILE:CG2	1:B:2108:LEU:HB2	2.46	0.45
1:B:2388:HIS:N	1:B:2389:PRO:CD	2.79	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.79	0.45
1:B:2547:PRO:HB3	1:B:2553:GLU:OE1	2.16	0.45
1:B:2464:ASN:HA	1:B:2464:ASN:HD22	1.61	0.45
1:B:2383:THR:HA	1:B:2386:HIS:HD2	1.80	0.45
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.99	0.45
1:B:2088:THR:HA	6:B:2702:BOG:H1'2	1.98	0.45
1:B:2131:ASN:ND2	1:B:2134:TYR:H	2.15	0.45
1:B:2397:ILE:HD12	1:B:2422:PHE:CE1	2.52	0.45
1:A:61:ARG:NH1	1:B:2542:PRO:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2362:ASP:HB3	1:B:2365:LEU:HG	1.99	0.45
1:B:2226:HIS:HA	1:B:2377:ILE:HD12	1.98	0.45
1:A:459:LYS:HB3	1:A:459:LYS:HE2	1.63	0.45
1:B:2073:GLU:O	1:B:2076:THR:HB	2.16	0.45
1:B:2120:ARG:HD2	1:B:2120:ARG:HA	1.81	0.45
1:A:276:PRO:HG2	1:A:279:ILE:HD11	1.98	0.45
1:B:2298:LEU:HA	1:B:2298:LEU:HD12	1.86	0.45
1:B:2252:LEU:O	1:B:2310:GLN:NE2	2.49	0.44
1:B:2294:LEU:HB3	1:B:2409:TYR:CD2	2.51	0.44
1:A:419:LEU:O	1:A:423:VAL:HG23	2.16	0.44
1:A:306:LEU:HD23	1:A:306:LEU:C	2.37	0.44
1:B:2226:HIS:CA	1:B:2377:ILE:HD12	2.47	0.44
1:B:2240:ARG:NH2	1:B:2273:MET:HE1	2.32	0.44
1:A:61:ARG:NH2	8:A:3003:HOH:O	2.49	0.44
1:A:78:ILE:O	1:A:82:LEU:HD13	2.17	0.44
1:B:2276:PRO:HD2	1:B:2279:ILE:HD13	1.98	0.44
1:B:2293:GLY:HA2	1:B:2299:MET:HE1	1.97	0.44
4:A:672:NAG:C6	4:A:673:MAN:C1	2.96	0.44
4:B:2672:NAG:C6	4:B:2673:MAN:C1	2.95	0.44
1:B:2178:LEU:HD22	1:B:2183:LEU:HG	1.99	0.44
1:A:249:ASP:OD2	1:A:317:LYS:HE2	2.18	0.44
1:B:2308:GLU:OE1	1:B:2311:ARG:NH1	2.51	0.44
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.99	0.44
1:B:2180:LYS:HD3	1:B:2490:GLU:OE2	2.17	0.44
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.48	0.44
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.53	0.44
1:B:2459:LYS:HB3	1:B:2459:LYS:HE2	1.63	0.44
1:B:2216:ARG:HH11	4:B:2672:NAG:C7	2.27	0.43
1:B:2203:GLN:CG	1:B:2298:LEU:HD11	2.48	0.43
1:A:294:LEU:HD23	1:A:295:VAL:CG2	2.48	0.43
1:A:105(A):ILE:O	1:A:108:LEU:N	2.51	0.43
1:B:2405:LYS:HD2	8:B:3692:HOH:O	2.17	0.43
1:B:2088:THR:HG23	6:B:2702:BOG:H3'2	1.99	0.43
1:B:2266:VAL:HG23	1:B:2284:GLN:O	2.17	0.43
1:A:362:ASP:HB3	1:A:365:LEU:HG	2.00	0.43
1:B:2043:ASN:O	1:B:2044:ARG:HB2	2.18	0.43
1:B:2303:THR:O	1:B:2307:ARG:HD3	2.19	0.43
1:A:124:ILE:HB	8:A:3495:HOH:O	2.18	0.43
1:A:542:PRO:O	1:B:2061:ARG:NH1	2.51	0.43
1:B:2034:ASN:HD22	1:B:2035:PRO:N	2.16	0.43
1:A:34:ASN:HD22	1:A:35:PRO:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2073:GLU:O	1:B:2074:PHE:C	2.56	0.43
1:B:2214:HIS:HD2	8:B:3233:HOH:O	2.02	0.43
1:B:2100:TRP:HA	1:B:2100:TRP:CE3	2.53	0.43
8:A:3106:HOH:O	1:B:2543:GLN:HB2	2.17	0.43
1:A:226:HIS:CA	1:A:377:ILE:HD12	2.48	0.43
1:A:247:PHE:C	1:A:248:LYS:HG2	2.39	0.43
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.19	0.43
1:B:2344:VAL:O	1:B:2349:VAL:HG23	2.19	0.43
1:A:553:GLU:HA	1:A:553:GLU:OE1	2.19	0.43
1:A:118:THR:HG22	1:A:369:GLN:HG2	2.00	0.43
1:B:2538:PRO:HD3	8:B:3638:HOH:O	2.17	0.43
1:B:2271:VAL:CG2	1:B:2273:MET:HE3	2.50	0.42
1:A:179:GLU:O	1:A:185:ARG:NH2	2.51	0.42
1:B:2087:ASN:HB3	6:B:2702:BOG:H3	2.01	0.42
1:B:2222:ARG:HD3	8:B:3289:HOH:O	2.19	0.42
1:A:276:PRO:HG2	1:A:279:ILE:HG13	2.01	0.42
1:B:2306:LEU:C	1:B:2306:LEU:HD23	2.38	0.42
1:B:105(B):ILE:O	1:B:2108:LEU:N	2.52	0.42
1:B:105(B):ILE:CD1	1:B:2108:LEU:HD12	2.48	0.42
1:B:2083:LYS:HE3	8:B:3661:HOH:O	2.18	0.42
1:A:131:ASN:HD22	1:A:134:TYR:H	1.67	0.42
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.49	0.42
1:B:2118:THR:HG22	1:B:2369:GLN:HG2	2.01	0.42
1:B:2160:PRO:HG2	1:B:2165:VAL:HA	2.01	0.42
1:A:396:ASN:H	1:A:429:GLN:NE2	2.15	0.42
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.82	0.42
1:A:183:LEU:O	1:A:438:ARG:HB3	2.20	0.42
1:A:400:GLN:HB2	1:A:402:TYR:CE2	2.55	0.42
1:A:283:LEU:HD21	1:A:415:LEU:HD12	2.02	0.42
1:A:275:TYR:HD2	1:A:279:ILE:HD12	1.84	0.42
1:A:464:ASN:ND2	1:A:475:TYR:H	2.11	0.42
1:A:294:LEU:HA	1:A:409:TYR:CD2	2.55	0.42
1:B:2470:PHE:CD2	1:B:2525:LEU:HD22	2.53	0.42
1:A:216:ARG:HH12	4:A:671:NAG:H3	1.84	0.42
1:A:398:GLU:HB3	1:A:399:ASP:H	1.68	0.42
1:A:280:PRO:HG2	1:A:283:LEU:HB2	2.02	0.42
1:B:2513:ARG:HD2	8:B:3249:HOH:O	2.19	0.42
1:B:2553:GLU:HA	1:B:2553:GLU:OE1	2.18	0.42
1:A:402:TYR:HA	1:A:406:GLN:OE1	2.20	0.42
1:A:259:GLY:N	8:A:3216:HOH:O	2.53	0.42
1:A:539:ILE:HA	1:A:544:TYR:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2096:PHE:HB3	1:B:2099:VAL:HG13	2.01	0.41
1:B:2261:VAL:O	1:B:2307:ARG:NH1	2.50	0.41
1:A:276:PRO:HD2	1:A:279:ILE:HD12	2.02	0.41
1:B:2308:GLU:CD	1:B:2311:ARG:HH11	2.23	0.41
1:B:2464:ASN:ND2	1:B:2475:TYR:H	2.10	0.41
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.84	0.41
1:B:2382:ASN:HD21	6:B:2704:BOG:H61	1.84	0.41
1:B:2082:LEU:N	1:B:2082:LEU:HD12	2.36	0.41
1:A:175:LYS:HG3	8:A:3497:HOH:O	2.20	0.41
1:B:2074:PHE:O	1:B:2077:ARG:HB2	2.20	0.41
1:B:2500:VAL:CG1	1:B:2500:VAL:O	2.68	0.41
1:A:96:PHE:HB3	1:A:99:VAL:HG13	2.01	0.41
1:A:253:LYS:HD3	8:A:3621:HOH:O	2.21	0.41
1:B:2554:VAL:HB	8:B:3346:HOH:O	2.19	0.41
1:A:322:GLU:HG3	1:A:322:GLU:H	1.47	0.41
1:A:308:GLU:CD	1:A:311:ARG:HH11	2.24	0.41
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.55	0.41
1:A:131:ASN:ND2	1:A:131:ASN:C	2.72	0.41
1:A:290:GLU:H	1:A:290:GLU:HG3	1.40	0.41
1:A:87:ASN:HB3	6:A:702:BOG:H3	2.03	0.41
1:A:470:PHE:CD2	1:A:525:LEU:HD22	2.56	0.41
1:B:2179:GLU:O	1:B:2185:ARG:NH2	2.54	0.41
1:B:2173:ASP:O	1:B:2177:VAL:HG23	2.21	0.41
1:A:444:VAL:O	1:A:444:VAL:CG1	2.69	0.41
1:B:2206:THR:HG21	1:B:2385:TYR:CE2	2.55	0.41
1:A:386:HIS:CE1	6:A:704:BOG:H1'2	2.56	0.40
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.86	0.40
1:B:2168:ASN:C	1:B:2170:GLU:N	2.74	0.40
1:B:2131:ASN:HD22	1:B:2134:TYR:H	1.69	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:B:2185:ARG:HE	1:B:2438:ARG:HD3	1.86	0.40
1:B:2092:ILE:HA	1:B:2096:PHE:HE1	1.86	0.40
1:A:168:ASN:C	1:A:170:GLU:N	2.74	0.40
1:A:582:VAL:O	1:A:583:GLN:C	2.60	0.40
1:B:2183:LEU:HA	1:B:2183:LEU:HD23	1.84	0.40
1:A:388:HIS:C	1:A:390:LEU:N	2.75	0.40
1:A:344:VAL:O	1:A:349:VAL:HG23	2.22	0.40
1:B:2452:ILE:O	1:B:2456:ARG:HG3	2.21	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	550/552 (100%)	522 (95%)	24 (4%)	4 (1%)	26	38
1	B	550/552 (100%)	516 (94%)	30 (6%)	4 (1%)	26	38
2	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1107/1113 (100%)	1045 (94%)	54 (5%)	8 (1%)	26	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	B	2121	SER
1	B	2122	TYR
1	A	514	PRO
1	B	2514	PRO
1	A	398	GLU
1	B	2435	ALA

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	492/492 (100%)	445 (90%)	47 (10%)	10	15
1	B	492/492 (100%)	442 (90%)	50 (10%)	9	13
2	F	7/7 (100%)	6 (86%)	1 (14%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	991/991 (100%)	893 (90%)	98 (10%)	10 14

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	54	GLN
1	A	56	LYS
1	A	93	LEU
1	A	99	VAL
1	A	101	ASN
1	A	117	LEU
1	A	120	ARG
1	A	123	LEU
1	A	131	ASN
1	A	137	LYS
1	A	171	LEU
1	A	178	LEU
1	A	203	GLN
1	A	230	LEU
1	A	238	LEU
1	A	239	ASP
1	A	252	LEU
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL
1	A	294	LEU
1	A	295	VAL
1	A	298	LEU
1	A	300	MET
1	A	310	GLN
1	A	311	ARG
1	A	322	GLU
1	A	352	LEU
1	A	369	GLN
1	A	377	ILE
1	A	385	TYR
1	A	406	GLN
1	A	408	LEU
1	A	412	SER
1	A	416	GLU
1	A	419	LEU

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Mol	Chain	Res	Type
1	A	422	PHE
1	A	444	VAL
1	A	459	LYS
1	A	484	GLU
1	A	509	VAL
1	A	525	LEU
1	A	534	LEU
1	A	543	GLN
1	A	579	SER
1	A	583	GLN
1	B	2034	ASN
1	B	2054	GLN
1	B	2056	LYS
1	B	2093	LEU
1	B	2099	VAL
1	B	2101	ASN
1	B	2117	LEU
1	B	2120	ARG
1	B	2123	LEU
1	B	2131	ASN
1	B	2137	LYS
1	B	2171	LEU
1	B	2178	LEU
1	B	2180	LYS
1	B	2230	LEU
1	B	2238	LEU
1	B	2239	ASP
1	B	2248	LYS
1	B	2252	LEU
1	B	2272	GLU
1	B	2289	GLN
1	B	2290	GLU
1	B	2291	VAL
1	B	2294	LEU
1	B	2298	LEU
1	B	2300	MET
1	B	2310	GLN
1	B	2311	ARG
1	B	2322	GLU
1	B	2352	LEU
1	B	2369	GLN
1	B	2377	ILE

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Mol	Chain	Res	Type
1	B	2385	TYR
1	B	2397	ILE
1	B	2398	GLU
1	B	2406	GLN
1	B	2409	TYR
1	B	2412	SER
1	B	2416	GLU
1	B	2419	LEU
1	B	2422	PHE
1	B	2444	VAL
1	B	2459	LYS
1	B	2484	GLU
1	B	2509	VAL
1	B	2525	LEU
1	B	2534	LEU
1	B	2543	GLN
1	B	2579	SER
1	B	2583	GLN
2	F	2596	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	131	ASN
1	A	386	HIS
1	A	417	HIS
1	A	429	GLN
1	A	454	GLN
1	A	464	ASN
1	B	2034	ASN
1	B	2131	ASN
1	B	2242	HIS
1	B	2386	HIS
1	B	2400	GLN
1	B	2417	HIS
1	B	2429	GLN
1	B	2454	GLN
1	B	2464	ASN
2	F	2601	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

12 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	$\#\|Z\| > 2$
3	NAG	A	661	1,3	14,14,15	0.79	0	15,19,21	0.62	0
3	NAG	A	662	3	14,14,15	0.90	0	15,19,21	0.83	0
4	NAG	A	671	1,4	14,14,15	0.37	0	15,19,21	0.67	0
4	NAG	A	672	4	14,14,15	2.13	2 (14%)	15,19,21	3.00	4 (26%)
4	MAN	A	673	4	11,11,12	1.29	2 (18%)	14,15,17	1.74	3 (21%)
4	MAN	A	674	4	11,11,12	2.28	3 (27%)	14,15,17	1.26	2 (14%)
3	NAG	B	2661	1,3	14,14,15	0.82	0	15,19,21	0.64	0
3	NAG	B	2662	3	14,14,15	0.86	0	15,19,21	0.85	0
4	NAG	B	2671	1,4	14,14,15	0.66	0	15,19,21	0.89	0
4	NAG	B	2672	4	14,14,15	1.33	2 (14%)	15,19,21	2.68	5 (33%)
4	MAN	B	2673	4	11,11,12	1.10	1 (9%)	14,15,17	1.61	3 (21%)
4	MAN	B	2674	4	11,11,12	2.30	3 (27%)	14,15,17	1.32	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	662	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	672	4	-	0/6/23/26	0/1/1/1
4	MAN	A	673	4	-	0/2/19/22	0/1/1/1
4	MAN	A	674	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	B	2661	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2662	3	-	0/6/23/26	0/1/1/1
4	NAG	B	2671	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2672	4	-	0/6/23/26	0/1/1/1
4	MAN	B	2673	4	-	0/2/19/22	0/1/1/1
4	MAN	B	2674	4	1/1/4/5	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	672	NAG	C1-C2	-4.48	1.46	1.52
4	B	2672	NAG	C1-C2	-2.30	1.49	1.52
4	A	673	MAN	C1-C2	2.12	1.57	1.52
4	B	2673	MAN	C6-C5	2.17	1.59	1.51
4	A	673	MAN	C6-C5	2.40	1.60	1.51
4	A	674	MAN	O5-C5	3.12	1.50	1.43
4	B	2674	MAN	O5-C5	3.45	1.51	1.43
4	B	2672	NAG	C8-C7	3.51	1.57	1.50
4	A	674	MAN	C4-C5	3.89	1.61	1.53
4	B	2674	MAN	C4-C5	3.90	1.61	1.53
4	B	2674	MAN	C2-C3	4.79	1.59	1.52
4	A	674	MAN	C2-C3	5.00	1.59	1.52
4	A	672	NAG	C8-C7	5.99	1.62	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	672	NAG	C8-C7-N2	-9.42	98.08	116.11
4	B	2672	NAG	C8-C7-N2	-7.94	100.90	116.11
4	B	2672	NAG	O7-C7-C8	-4.93	113.02	122.06
4	A	672	NAG	O7-C7-C8	-4.81	113.23	122.06
4	A	672	NAG	C2-N2-C7	-2.85	119.38	123.04
4	A	672	NAG	C3-C2-N2	-2.77	103.93	110.56
4	A	674	MAN	O2-C2-C1	-2.45	104.29	109.21
4	B	2672	NAG	C2-N2-C7	-2.40	119.95	123.04
4	B	2674	MAN	O2-C2-C1	-2.36	104.47	109.21
4	B	2672	NAG	C3-C2-N2	-2.32	104.99	110.56
4	A	673	MAN	O5-C1-C2	2.40	114.75	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2672	NAG	C1-O5-C5	2.47	115.38	112.25
4	A	674	MAN	O5-C1-C2	2.77	115.35	110.86
4	B	2673	MAN	O5-C1-C2	2.82	115.44	110.86
4	B	2673	MAN	O6-C6-C5	2.97	121.14	111.33
4	A	673	MAN	O6-C6-C5	3.01	121.28	111.33
4	B	2674	MAN	O5-C1-C2	3.12	115.92	110.86
4	B	2673	MAN	C1-O5-C5	3.55	116.75	112.25
4	A	673	MAN	C1-O5-C5	4.44	117.89	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2674	MAN	C1
4	A	674	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	671	NAG	1	0
4	A	672	NAG	2	0
4	A	673	MAN	2	0
4	B	2672	NAG	5	0
4	B	2673	MAN	2	0

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	681	1	14,14,15	0.86	1 (7%)	15,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	ACD	A	701	-	18,21,21	0.75	0	18,21,21	0.59	0
6	BOG	A	702	-	20,20,20	0.82	1 (5%)	25,25,25	0.71	0
6	BOG	A	703	-	20,20,20	0.89	0	25,25,25	0.72	1 (4%)
6	BOG	A	704	-	20,20,20	0.90	2 (10%)	25,25,25	0.67	0
5	NAG	B	2681	1	14,14,15	0.80	0	15,19,21	0.94	1 (6%)
7	ACD	B	2701	-	18,21,21	0.58	0	18,21,21	0.52	0
6	BOG	B	2702	-	20,20,20	0.66	0	25,25,25	0.64	0
6	BOG	B	2704	-	20,20,20	0.82	2 (10%)	25,25,25	0.67	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
5	NAG	A	681	1	-	0/6/23/26	0/1/1/1
7	ACD	A	701	-	-	0/17/19/19	0/0/0/0
6	BOG	A	702	-	-	0/11/31/31	0/1/1/1
6	BOG	A	703	-	-	0/11/31/31	0/1/1/1
6	BOG	A	704	-	-	0/11/31/31	0/1/1/1
5	NAG	B	2681	1	-	0/6/23/26	0/1/1/1
7	ACD	B	2701	-	-	0/17/19/19	0/0/0/0
6	BOG	B	2702	-	-	0/11/31/31	0/1/1/1
6	BOG	B	2704	-	-	0/11/31/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	BOG	O5-C1	2.03	1.47	1.41
6	B	2704	BOG	O1-C1	2.10	1.43	1.40
6	B	2704	BOG	O5-C1	2.21	1.47	1.41
6	A	704	BOG	O1-C1	2.29	1.44	1.40
5	A	681	NAG	C1-C2	2.30	1.55	1.52
6	A	704	BOG	O5-C1	2.33	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2681	NAG	C8-C7-N2	-2.37	111.56	116.11
6	A	703	BOG	O1-C1-C2	2.05	110.63	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	BOG	1	0
6	A	703	BOG	3	0
6	A	704	BOG	2	0
6	B	2702	BOG	3	0
6	B	2704	BOG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	552/552 (100%)	-0.32	13 (2%)	62	61	14, 26, 43, 56	0
1	B	552/552 (100%)	-0.24	15 (2%)	58	57	12, 27, 46, 61	0
2	F	9/9 (100%)	2.33	5 (55%)	0	0	52, 55, 66, 71	0
All	All	1113/1113 (100%)	-0.26	33 (2%)	54	53	12, 27, 46, 71	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2409	TYR	7.3
2	F	2603	SER	6.9
1	B	2583	GLN	4.1
1	B	2074	PHE	3.9
1	A	74	PHE	3.8
2	F	2600	ILE	3.4
2	F	2601	ASN	3.0
2	F	2599	THR	3.0
1	A	399	ASP	3.0
1	B	2081	LEU	2.8
1	A	75	LEU	2.7
1	A	80	LEU	2.6
1	B	2399	ASP	2.6
1	B	2274	ILE	2.6
1	B	2065	TYR	2.5
1	A	409	TYR	2.4
1	A	102	ILE	2.4
1	B	2214	HIS	2.4
1	B	2075	LEU	2.4
1	A	122	TYR	2.4
1	B	2078	ILE	2.3
1	B	2077	ARG	2.3
1	B	2406	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	107	PHE	2.3
1	A	583	GLN	2.3
1	A	33	ALA	2.2
1	B	2294	LEU	2.2
1	A	52	PHE	2.2
1	B	2272	GLU	2.1
2	F	2595	THR	2.1
1	A	421	GLN	2.0
1	A	77	ARG	2.0
1	B	2053	ASP	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)

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
3	NAG	A	661	14/15	0.86	0.23	5.61	44,50,53,58	0
3	NAG	B	2661	14/15	0.66	0.35	5.56	52,54,58,64	0
4	NAG	A	672	14/15	0.80	0.36	2.39	46,52,55,57	0
4	NAG	A	671	14/15	0.95	0.13	0.33	28,30,33,39	0
4	NAG	B	2671	14/15	0.94	0.15	0.19	27,29,34,41	0
3	NAG	B	2662	14/15	0.63	0.70	-	68,71,74,75	0
4	NAG	B	2672	14/15	0.78	0.36	-	49,55,57,62	0
4	MAN	A	673	11/12	0.58	0.40	-	60,62,65,67	0
4	MAN	B	2674	11/12	0.38	0.78	-	78,80,82,82	0
4	MAN	A	674	11/12	0.66	0.43	-	70,71,72,72	0
3	NAG	A	662	14/15	0.65	0.48	-	64,67,70,72	0
4	MAN	B	2673	11/12	0.54	0.42	-	66,67,72,76	0

6.4 Ligands

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
6	BOG	A	702	20/20	0.81	0.30	5.06	38,50,54,54	0
5	NAG	B	2681	14/15	0.66	0.46	3.96	68,70,71,72	0
6	BOG	A	704	20/20	0.57	0.35	3.68	42,63,65,67	0
5	NAG	A	681	14/15	0.79	0.42	3.54	58,61,64,66	0
6	BOG	B	2702	20/20	0.85	0.28	3.23	40,45,47,47	0
6	BOG	B	2704	20/20	0.77	0.25	1.82	32,61,64,65	0
6	BOG	A	703	20/20	0.86	0.17	1.34	33,44,46,47	0
7	ACD	A	701	22/22	0.95	0.17	0.80	18,22,28,31	0
7	ACD	B	2701	22/22	0.95	0.15	0.26	19,25,29,32	0

6.5 Other polymers

There are no such residues in this entry.