Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:43 AM GMT

PDB ID	:	2ICF
Title	:	CRIg bound to C3b
Authors	:	Wiesmann, C.
Deposited on	:	2006-09-12
Resolution	:	4.10 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:

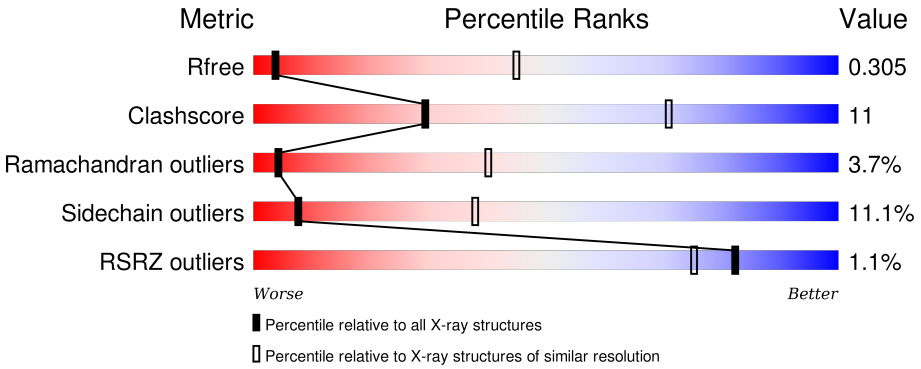
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.10 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	642	63% 31% 5%
2	B	915	% 68% 27%
3	S	119	3% 71% 26%

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
4	NAG	A	643	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13236 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5008	3188	848	957	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	1161	0	0
			7213	4572	1213	1390	38			

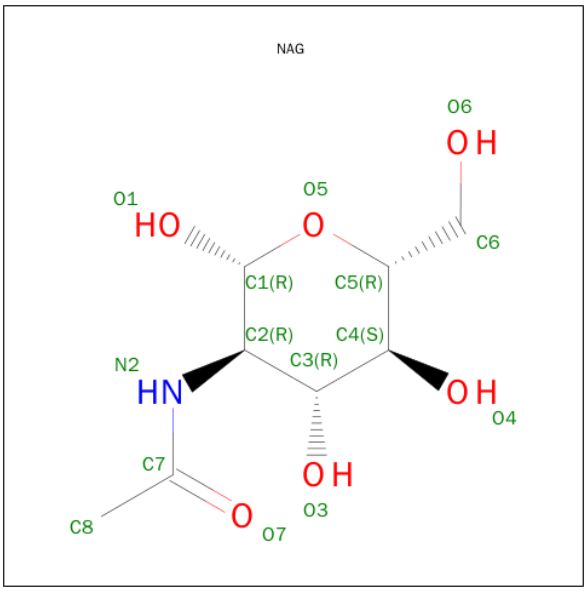
- Molecule 3 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			

- 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		

- 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	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

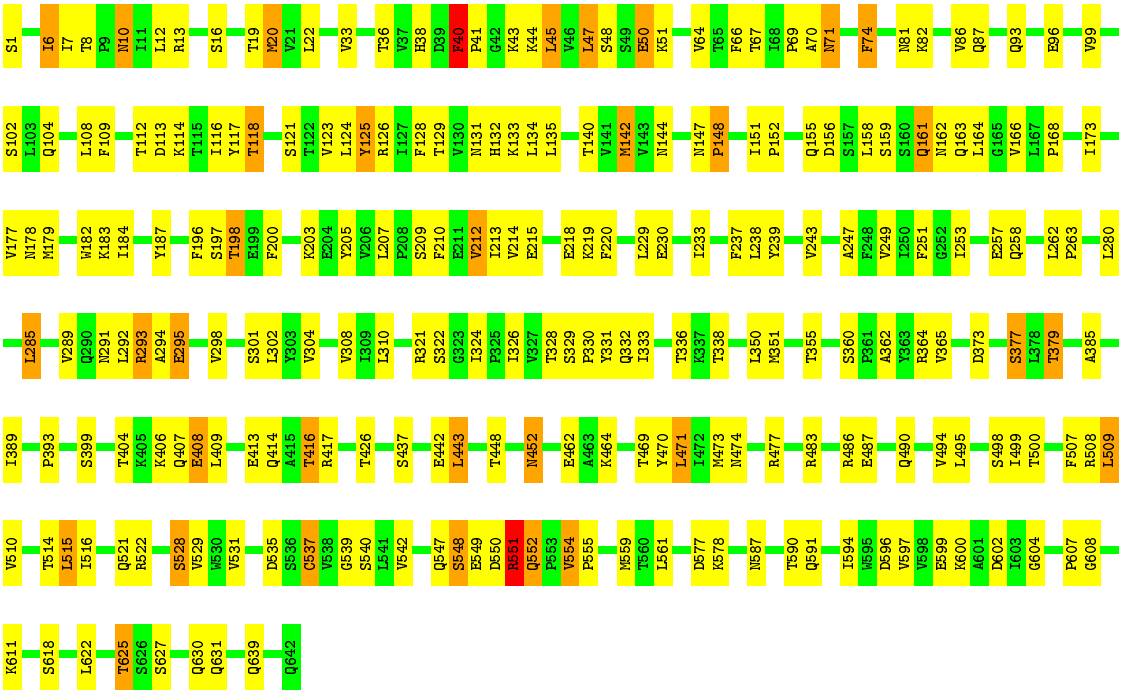
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0

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.

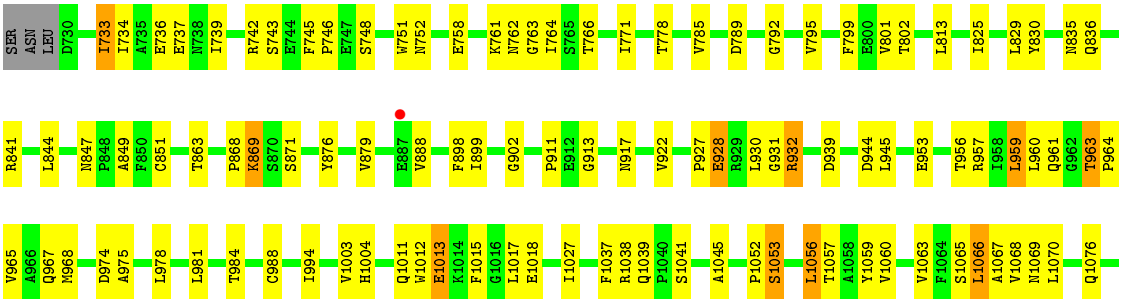
- Molecule 1: Complement C3 beta chain

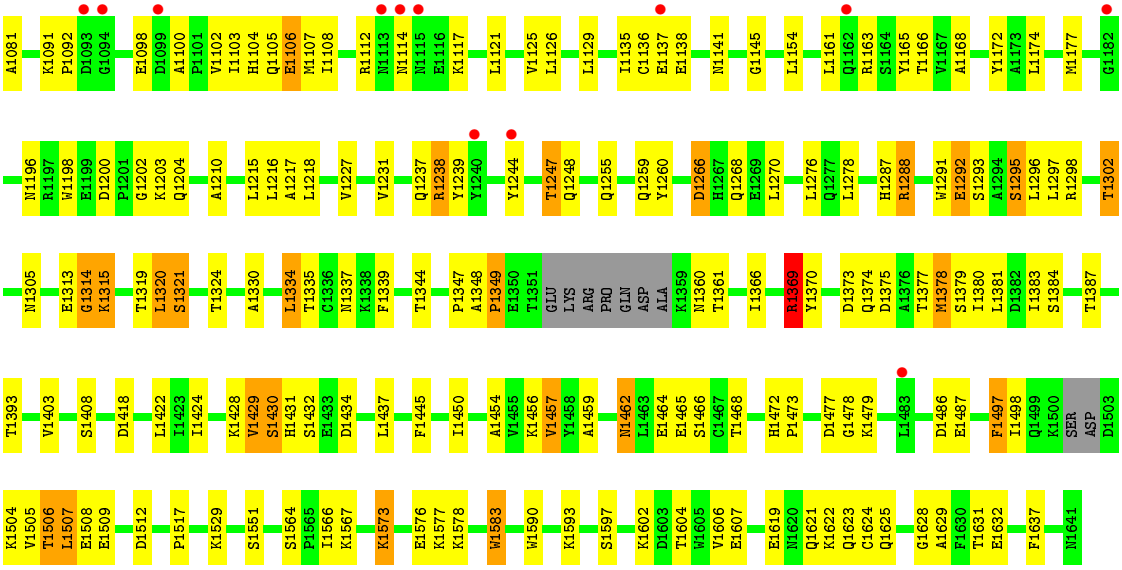
Chain A:



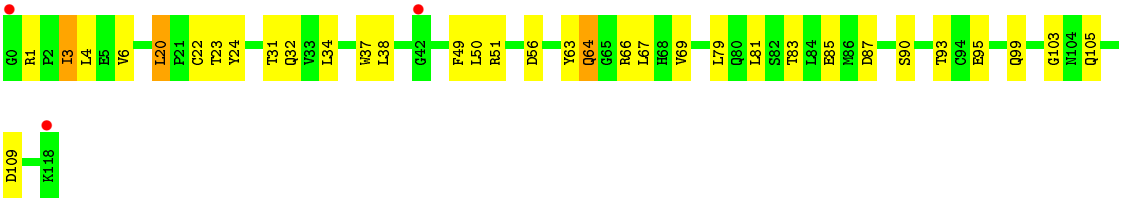
- Molecule 2: Complement C3 alpha chain

Chain B:





- Molecule 3: V-set and immunoglobulin domain-containing protein 4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.61Å 255.75Å 180.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 19.98 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-4.10) 96.0 (19.98-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.252 , 0.330 0.236 , 0.305	Depositor DCC
R_{free} test set	875 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	157.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 133.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 17204 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: CA, BMA, NAG

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	0.58	0/5108	0.71	0/6939
2	B	0.59	5/7356 (0.1%)	0.82	1/9958 (0.0%)
3	S	0.61	0/972	0.66	0/1323
All	All	0.59	5/13436 (0.0%)	0.77	1/18220 (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	2
2	B	0	7
4	A	1	0
All	All	1	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1041	SER	CB-OG	12.37	1.58	1.42
2	B	1607	GLU	CD-OE2	9.88	1.36	1.25
2	B	737	GLU	CD-OE1	6.90	1.33	1.25
2	B	737	GLU	CD-OE2	6.34	1.32	1.25
2	B	1053	SER	CB-OG	6.15	1.50	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1497	PHE	O-C-N	-49.53	43.45	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	643	NAG	C1

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	PHE	Peptide
1	A	599	GLU	Peptide
2	B	1056	LEU	Mainchain
2	B	1335	THR	Peptide
2	B	1347	PRO	Peptide
2	B	1369	ARG	Peptide
2	B	1430	SER	Peptide
2	B	1497	PHE	Mainchain
2	B	930	LEU	Peptide

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	5008	0	5071	143	0
2	B	7213	0	7141	123	99
3	S	950	0	935	15	0
4	A	50	0	43	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
All	All	13236	0	13203	274	99

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 11.

All (274) 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:B:1370:TYR:N	2:B:1430:SER:O	2.13	0.81
1:A:507:PHE:CE1	1:A:531:VAL:HB	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1383:ILE:HD11	2:B:1424:ILE:HD11	1.69	0.73
1:A:214:VAL:HG12	1:A:233:ILE:HD13	1.70	0.73
2:B:1330:ALA:HB1	2:B:1334:LEU:HD21	1.74	0.69
3:S:4:LEU:HD22	3:S:22:CYS:SG	2.33	0.69
1:A:487:GLU:O	1:A:490:GLN:NE2	2.26	0.69
1:A:123:VAL:HG23	1:A:173:ILE:HD11	1.73	0.68
2:B:1059:TYR:O	2:B:1063:VAL:HG23	1.94	0.68
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.29	0.67
1:A:329:SER:OG	1:A:413:GLU:O	2.04	0.67
2:B:785:VAL:HG22	2:B:795:VAL:HG22	1.75	0.66
1:A:302:LEU:HG	1:A:326:ILE:HD11	1.77	0.66
1:A:362:ALA:O	1:A:379:THR:HG21	1.96	0.66
2:B:956:THR:HG23	2:B:1324:THR:CG2	2.29	0.63
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.34	0.62
1:A:443:LEU:HD22	1:A:499:ILE:HG21	1.82	0.62
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.35	0.62
1:A:144:ASN:HD21	1:A:155:GLN:HE21	1.46	0.61
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.36	0.61
2:B:1369:ARG:HG2	2:B:1430:SER:O	2.01	0.61
1:A:229:LEU:HD21	1:A:324:ILE:HD13	1.82	0.60
1:A:302:LEU:CG	1:A:326:ILE:HD11	2.32	0.60
1:A:293:ARG:HG2	1:A:293:ARG:O	2.02	0.60
1:A:197:SER:O	1:A:198:THR:OG1	2.14	0.60
1:A:45:LEU:HD12	1:A:48:SER:HB2	1.82	0.59
2:B:956:THR:HA	2:B:1324:THR:HG22	1.85	0.59
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.38	0.59
2:B:1348:ALA:HB1	2:B:1349:PRO:CD	2.33	0.59
1:A:220:PHE:CE2	1:A:330:PRO:HB3	2.38	0.59
3:S:6:VAL:HG22	3:S:22:CYS:HA	1.84	0.58
1:A:40:PHE:CD2	1:A:41:PRO:HD3	2.38	0.58
1:A:142:MET:HB2	1:A:187:TYR:CE1	2.38	0.57
2:B:1381:LEU:HB2	2:B:1424:ILE:HB	1.87	0.57
2:B:1297:LEU:HD23	2:B:1298:ARG:N	2.20	0.56
2:B:1348:ALA:HB1	2:B:1349:PRO:HD2	1.86	0.56
2:B:1126:LEU:HD21	2:B:1177:MET:CE	2.35	0.56
1:A:522:ARG:HB3	1:A:630:GLN:HE22	1.69	0.56
1:A:253:ILE:N	1:A:253:ILE:HD12	2.21	0.56
1:A:470:TYR:CZ	1:A:495:LEU:HD21	2.41	0.56
1:A:338:THR:OG1	1:A:351:MET:N	2.38	0.56
1:A:509:LEU:O	1:A:528:SER:HA	2.05	0.56
2:B:1377:THR:O	2:B:1378:MET:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:O	1:A:134:LEU:N	2.39	0.55
1:A:262:LEU:O	1:A:263:PRO:C	2.44	0.55
2:B:1472:HIS:ND1	2:B:1473:PRO:HD2	2.21	0.55
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.89	0.55
2:B:742:ARG:N	2:B:902:GLY:O	2.38	0.55
2:B:1373:ASP:OD1	2:B:1430:SER:OG	2.24	0.54
1:A:125:TYR:CD1	1:A:184:ILE:HD13	2.42	0.54
1:A:40:PHE:CG	1:A:41:PRO:HD3	2.42	0.54
1:A:36:THR:HB	1:A:87:GLN:HB3	1.90	0.54
2:B:733:ILE:HG23	2:B:734:ILE:N	2.23	0.54
2:B:978:LEU:HB3	2:B:981:LEU:HD12	1.89	0.54
2:B:927:PRO:O	2:B:928:GLU:HB2	2.07	0.54
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.89	0.54
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.43	0.53
2:B:868:PRO:O	2:B:869:LYS:C	2.47	0.53
2:B:898:PHE:O	2:B:899:ILE:HD13	2.08	0.53
2:B:1464:GLU:O	2:B:1466:SER:N	2.41	0.53
2:B:1276:LEU:N	2:B:1276:LEU:HD12	2.23	0.53
2:B:1456:LYS:HB2	2:B:1468:THR:HG23	1.91	0.53
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.90	0.53
2:B:1237:GLN:O	2:B:1239:TYR:N	2.42	0.53
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.91	0.52
1:A:452:ASN:HD22	1:A:452:ASN:N	2.08	0.52
1:A:522:ARG:O	1:A:630:GLN:NE2	2.41	0.52
1:A:469:THR:HG23	1:A:483:ARG:HD3	1.89	0.52
2:B:1477:ASP:O	2:B:1479:LYS:N	2.42	0.52
2:B:1369:ARG:HG3	2:B:1429:VAL:HG23	1.92	0.52
1:A:81:ASN:HD22	1:A:81:ASN:N	2.05	0.52
1:A:596:ASP:O	1:A:600:LYS:N	2.44	0.51
1:A:591:GLN:O	1:A:594:ILE:HB	2.10	0.51
2:B:1288:ARG:O	2:B:1298:ARG:NH1	2.43	0.51
1:A:118:THR:O	1:A:121:SER:OG	2.20	0.51
3:S:63:TYR:O	3:S:64:GLN:C	2.48	0.51
2:B:1053:SER:HA	2:B:1100:ALA:HB3	1.93	0.51
1:A:237:PHE:O	1:A:239:TYR:N	2.43	0.51
2:B:1295:SER:OG	2:B:1297:LEU:N	2.42	0.50
1:A:102:SER:HB2	1:A:104:GLN:HE21	1.76	0.50
3:S:24:TYR:OH	3:S:32:GLN:NE2	2.42	0.50
2:B:1154:LEU:HB2	2:B:1174:LEU:HD21	1.94	0.50
1:A:443:LEU:CD2	1:A:499:ILE:HG21	2.41	0.50
1:A:289:VAL:HG13	1:A:291:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ASP:OD2	1:A:604:GLY:N	2.32	0.50
1:A:331:TYR:CE1	1:A:365:VAL:HG21	2.47	0.50
1:A:377:SER:OG	1:A:385:ALA:HB1	2.12	0.50
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.93	0.49
1:A:594:ILE:O	1:A:597:VAL:N	2.45	0.49
1:A:86:VAL:O	1:A:96:GLU:HA	2.13	0.49
2:B:961:GLN:HB3	2:B:1319:THR:HB	1.94	0.49
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.47	0.49
2:B:1369:ARG:HD3	2:B:1434:ASP:HA	1.95	0.49
2:B:1098:GLU:HB2	2:B:1121:LEU:HD21	1.94	0.49
2:B:1105:GLN:NE2	2:B:1108:ILE:HD13	2.28	0.49
1:A:220:PHE:CZ	1:A:330:PRO:HB3	2.48	0.49
1:A:45:LEU:HD23	1:A:45:LEU:H	1.78	0.49
1:A:289:VAL:O	1:A:289:VAL:HG12	2.12	0.49
2:B:1165:TYR:CD1	2:B:1210:ALA:HB2	2.48	0.49
3:S:37:TRP:CE3	3:S:93:THR:O	2.66	0.49
2:B:1168:ALA:HB2	2:B:1198:TRP:CD1	2.48	0.48
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.94	0.48
2:B:1107:MET:O	2:B:1248:GLN:HG2	2.13	0.48
1:A:561:LEU:HD13	2:B:771:ILE:HD11	1.95	0.48
2:B:1369:ARG:HB3	2:B:1431:HIS:HA	1.95	0.48
2:B:1320:LEU:C	2:B:1320:LEU:HD12	2.33	0.48
1:A:295:GLU:OE1	1:A:295:GLU:N	2.45	0.48
3:S:83:THR:O	3:S:83:THR:HG22	2.14	0.48
2:B:1141:ASN:N	2:B:1141:ASN:HD22	2.11	0.48
2:B:965:VAL:O	2:B:1268:GLN:HB2	2.14	0.48
2:B:1330:ALA:HB1	2:B:1334:LEU:CD2	2.43	0.48
1:A:416:THR:OG1	1:A:417:ARG:N	2.47	0.48
1:A:548:SER:O	1:A:550:ASP:N	2.47	0.48
1:A:113:ASP:CG	1:A:124:LEU:HD12	2.35	0.48
1:A:437:SER:OG	1:A:452:ASN:HB2	2.14	0.47
1:A:151:ILE:CG2	2:B:1297:LEU:HD13	2.43	0.47
2:B:931:GLY:O	2:B:932:ARG:HB2	2.13	0.47
1:A:486:ARG:HG3	1:A:490:GLN:NE2	2.30	0.47
1:A:40:PHE:HB3	1:A:41:PRO:HD3	1.96	0.47
1:A:550:ASP:O	1:A:551:ARG:HG2	2.15	0.47
1:A:177:VAL:HG22	1:A:178:ASN:N	2.29	0.47
2:B:844:LEU:HB2	2:B:876:TYR:CE1	2.50	0.47
1:A:123:VAL:CG2	1:A:173:ILE:HD11	2.43	0.47
1:A:285:LEU:C	1:A:285:LEU:HD12	2.36	0.47
1:A:212:VAL:O	1:A:213:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1266:ASP:N	2:B:1266:ASP:OD1	2.47	0.47
1:A:625:THR:HG23	1:A:631:GLN:CB	2.45	0.46
2:B:1057:THR:HG22	2:B:1081:ALA:HB1	1.96	0.46
2:B:1237:GLN:O	2:B:1238:ARG:C	2.54	0.46
1:A:7:ILE:HD12	1:A:7:ILE:N	2.30	0.46
1:A:74:PHE:O	1:A:82:LYS:NZ	2.48	0.46
2:B:1098:GLU:HB2	2:B:1121:LEU:CD2	2.46	0.46
2:B:743:SER:O	2:B:745:PHE:CD2	2.68	0.46
2:B:1291:TRP:O	2:B:1292:GLU:CB	2.64	0.46
1:A:164:LEU:O	1:A:166:VAL:HG23	2.15	0.46
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.98	0.45
1:A:551:ARG:HA	1:A:551:ARG:NH1	2.31	0.45
2:B:1172:TYR:HA	2:B:1217:ALA:HB2	1.98	0.45
1:A:537:CYS:HB3	1:A:539:GLY:O	2.16	0.45
1:A:114:LYS:N	1:A:117:TYR:OH	2.48	0.45
2:B:1045:ALA:HB2	2:B:1052:PRO:HA	1.98	0.45
1:A:151:ILE:HG21	2:B:1297:LEU:HD13	1.99	0.45
1:A:333:ILE:HD12	1:A:416:THR:HA	1.99	0.45
2:B:1004:HIS:CD2	2:B:1066:LEU:HD11	2.51	0.45
2:B:927:PRO:O	2:B:928:GLU:CB	2.63	0.45
1:A:470:TYR:CE1	1:A:495:LEU:HD21	2.51	0.45
2:B:851:CYS:CB	2:B:879:VAL:HB	2.47	0.45
2:B:829:LEU:HD12	2:B:829:LEU:N	2.32	0.45
2:B:945:LEU:HD12	2:B:1305:ASN:HD22	1.81	0.45
2:B:1370:TYR:O	2:B:1431:HIS:HB2	2.16	0.45
1:A:293:ARG:O	1:A:295:GLU:N	2.50	0.45
2:B:1102:VAL:HG22	2:B:1105:GLN:HE21	1.82	0.45
3:S:67:LEU:HD21	3:S:79:LEU:HD11	1.98	0.45
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.99	0.45
1:A:406:LYS:N	1:A:414:GLN:HE22	2.14	0.45
2:B:1278:LEU:H	2:B:1278:LEU:HD12	1.82	0.45
2:B:1003:VAL:HG21	2:B:1027:ILE:HD11	1.99	0.44
2:B:959:LEU:HB3	2:B:1321:SER:OG	2.17	0.44
1:A:40:PHE:CB	1:A:41:PRO:HD3	2.47	0.44
1:A:551:ARG:O	1:A:552:GLN:CB	2.65	0.44
1:A:407:GLN:O	1:A:408:GLU:CB	2.65	0.44
2:B:1381:LEU:HD23	2:B:1457:VAL:HG13	1.99	0.44
1:A:69:PRO:O	1:A:71:ASN:N	2.50	0.44
1:A:547:GLN:OE1	1:A:559:MET:HA	2.17	0.44
1:A:302:LEU:HB2	1:A:324:ILE:HB	2.00	0.44
1:A:197:SER:O	1:A:198:THR:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:37:TRP:HB2	3:S:49:PHE:HB3	2.00	0.44
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.52	0.44
1:A:182:TRP:HB3	1:A:200:PHE:CE2	2.53	0.44
2:B:1215:LEU:HD11	2:B:1231:VAL:HG23	1.99	0.44
2:B:961:GLN:HE21	2:B:963:THR:HG23	1.82	0.44
1:A:280:LEU:HD11	1:A:285:LEU:HB2	1.98	0.44
2:B:736:GLU:HA	2:B:739:ILE:HD12	2.00	0.44
1:A:135:LEU:HA	2:B:792:GLY:HA2	2.00	0.44
1:A:251:PHE:CD1	1:A:304:VAL:HG22	2.53	0.44
3:S:99:GLN:HG2	3:S:105:GLN:HG2	1.99	0.44
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.82	0.44
1:A:528:SER:OG	1:A:608:GLY:HA2	2.18	0.43
2:B:1384:SER:OG	2:B:1454:ALA:N	2.51	0.43
1:A:50:GLU:HB3	1:A:64:VAL:HG22	2.00	0.43
2:B:1293:SER:O	2:B:1293:SER:OG	2.32	0.43
2:B:1011:GLN:O	2:B:1012:TRP:C	2.56	0.43
1:A:365:VAL:H	1:A:379:THR:HG22	1.83	0.43
2:B:1037:PHE:O	2:B:1039:GLN:N	2.52	0.43
1:A:81:ASN:ND2	1:A:81:ASN:N	2.66	0.43
2:B:945:LEU:HD12	2:B:1305:ASN:ND2	2.33	0.43
2:B:1231:VAL:HG21	2:B:1260:TYR:CE1	2.53	0.43
2:B:761:LYS:O	2:B:762:ASN:HB2	2.19	0.43
1:A:40:PHE:CG	1:A:41:PRO:CD	3.02	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.19	0.43
1:A:126:ARG:HG3	2:B:751:TRP:HZ2	1.82	0.43
1:A:551:ARG:HA	1:A:551:ARG:CZ	2.48	0.43
1:A:529:VAL:O	1:A:529:VAL:HG13	2.19	0.43
1:A:12:LEU:HD11	1:A:99:VAL:HG11	2.01	0.43
1:A:295:GLU:O	1:A:298:VAL:HG23	2.19	0.43
2:B:745:PHE:N	2:B:746:PRO:CD	2.81	0.43
3:S:67:LEU:CG	3:S:79:LEU:HD11	2.49	0.43
1:A:507:PHE:CD1	1:A:531:VAL:HB	2.53	0.43
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.84	0.43
1:A:16:SER:O	1:A:67:THR:HA	2.19	0.43
2:B:1369:ARG:CZ	2:B:1430:SER:H	2.32	0.43
1:A:625:THR:HG23	1:A:631:GLN:HB2	2.01	0.43
2:B:1067:ALA:HA	2:B:1070:LEU:HG	2.01	0.43
1:A:152:PRO:CG	2:B:1295:SER:HA	2.49	0.42
2:B:1366:ILE:HD12	2:B:1437:LEU:HD11	2.01	0.42
2:B:1065:SER:O	2:B:1068:VAL:HG13	2.18	0.42
1:A:554:VAL:HG13	1:A:555:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:CE1	1:A:594:ILE:HG23	2.54	0.42
1:A:128:PHE:CD1	1:A:166:VAL:HG22	2.53	0.42
1:A:407:GLN:O	1:A:408:GLU:HB2	2.19	0.42
2:B:1291:TRP:O	2:B:1292:GLU:HB2	2.20	0.42
2:B:1293:SER:OG	2:B:1296:LEU:HD23	2.20	0.42
1:A:471:LEU:HD12	1:A:510:VAL:O	2.19	0.42
2:B:799:PHE:CE2	2:B:801:VAL:CG2	3.02	0.42
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.54	0.42
1:A:597:VAL:O	1:A:600:LYS:N	2.47	0.42
1:A:161:GLN:HE21	1:A:161:GLN:HB2	1.73	0.42
1:A:257:GLU:N	1:A:257:GLU:CD	2.73	0.42
2:B:1380:ILE:O	2:B:1457:VAL:HG12	2.20	0.42
3:S:20:LEU:HD12	3:S:79:LEU:HD23	2.02	0.42
2:B:1462:ASN:HD22	2:B:1462:ASN:HA	1.65	0.42
2:B:1293:SER:O	2:B:1296:LEU:HG	2.19	0.42
2:B:799:PHE:CE2	2:B:801:VAL:HG22	2.54	0.42
2:B:1125:VAL:O	2:B:1129:LEU:HG	2.20	0.42
1:A:515:LEU:HD12	1:A:516:ILE:C	2.41	0.42
1:A:590:THR:O	1:A:591:GLN:C	2.58	0.41
1:A:108:LEU:HD23	1:A:129:THR:HA	2.02	0.41
1:A:237:PHE:CD2	1:A:243:VAL:HG22	2.55	0.41
1:A:166:VAL:O	1:A:168:PRO:HD3	2.21	0.41
2:B:1011:GLN:O	2:B:1013:GLU:N	2.53	0.41
1:A:116:ILE:HD11	1:A:203:LYS:HB3	2.00	0.41
2:B:1204:GLN:HE21	2:B:1204:GLN:HB3	1.71	0.41
2:B:1218:LEU:HB3	2:B:1227:VAL:HG22	2.01	0.41
1:A:113:ASP:HB3	1:A:124:LEU:HB2	2.02	0.41
2:B:1068:VAL:HG11	2:B:1135:ILE:HD11	2.02	0.41
2:B:847:ASN:ND2	2:B:849:ALA:HB3	2.36	0.41
1:A:507:PHE:CE1	1:A:531:VAL:CB	3.00	0.41
2:B:1287:HIS:CE1	2:B:1298:ARG:HB3	2.55	0.41
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	2.03	0.41
3:S:38:LEU:HD12	3:S:38:LEU:N	2.36	0.41
3:S:3:ILE:HD12	3:S:3:ILE:N	2.36	0.41
2:B:763:GLY:O	2:B:764:ILE:HD13	2.20	0.41
1:A:355:THR:HB	1:A:360:SER:O	2.20	0.41
3:S:34:LEU:HD12	3:S:51:ARG:O	2.21	0.41
1:A:10:ASN:HA	1:A:10:ASN:HD22	1.64	0.41
2:B:745:PHE:N	2:B:746:PRO:HD3	2.36	0.41
1:A:218:GLU:C	1:A:220:PHE:H	2.24	0.41
1:A:253:ILE:HD11	1:A:262:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HG22	1:A:20:MET:N	2.36	0.41
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.56	0.41
3:S:69:VAL:HG22	3:S:79:LEU:HD12	2.02	0.41
1:A:332:GLN:HB3	1:A:355:THR:OG1	2.20	0.41
2:B:1314:GLY:O	2:B:1315:LYS:HB2	2.20	0.41
1:A:577:ASP:O	1:A:578:LYS:C	2.59	0.41
2:B:1161:LEU:HD13	2:B:1166:THR:HB	2.02	0.41
2:B:1369:ARG:HD3	2:B:1434:ASP:CA	2.51	0.41
2:B:813:LEU:HD21	2:B:888:VAL:HB	2.03	0.41
1:A:131:ASN:O	1:A:133:LYS:N	2.54	0.40
2:B:964:PRO:HB3	2:B:1270:LEU:HD11	2.02	0.40
1:A:362:ALA:O	1:A:379:THR:CG2	2.68	0.40
2:B:1379:SER:OG	2:B:1459:ALA:HA	2.21	0.40
1:A:473:MET:O	1:A:507:PHE:HA	2.21	0.40
2:B:956:THR:HB	2:B:1302:THR:HB	2.03	0.40
2:B:1126:LEU:HD21	2:B:1177:MET:HE1	2.02	0.40
2:B:1107:MET:O	2:B:1247:THR:HB	2.21	0.40
2:B:1057:THR:CG2	2:B:1081:ALA:HB1	2.51	0.40
2:B:1012:TRP:HB3	2:B:1017:LEU:HD12	2.02	0.40
1:A:10:ASN:ND2	1:A:622:LEU:O	2.53	0.40
1:A:38:HIS:CD2	1:A:43:LYS:HB3	2.57	0.40
1:A:117:TYR:CE1	1:A:123:VAL:HG22	2.57	0.40
1:A:302:LEU:HG	1:A:326:ILE:CD1	2.50	0.40
1:A:515:LEU:HD12	1:A:516:ILE:N	2.36	0.40
2:B:975:ALA:HB1	2:B:1015:PHE:HB2	2.03	0.40
2:B:960:LEU:HD23	2:B:960:LEU:HA	1.92	0.40

All (99) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1105:GLN:N	2:B:1508:GLU:CD[5_445]	0.40	1.80
2:B:1203:LYS:NZ	2:B:1622:LYS:C[5_445]	0.42	1.78
2:B:1203:LYS:C	2:B:1622:LYS:NZ[5_445]	0.70	1.50
2:B:1202:GLY:CA	2:B:1621:GLN:CG[5_445]	0.83	1.37
2:B:1203:LYS:CG	2:B:1622:LYS:CB[5_445]	0.90	1.30
2:B:1202:GLY:CA	2:B:1621:GLN:CB[5_445]	1.01	1.19
2:B:1105:GLN:N	2:B:1508:GLU:OE1[5_445]	1.03	1.17
2:B:1202:GLY:N	2:B:1621:GLN:CD[5_445]	1.05	1.15
2:B:1203:LYS:NZ	2:B:1623:GLN:N[5_445]	1.07	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1104:HIS:C	2:B:1508:GLU:CD[5_445]	1.08	1.12
2:B:1104:HIS:CA	2:B:1508:GLU:CG[5_445]	1.09	1.11
2:B:1203:LYS:CG	2:B:1622:LYS:CG[5_445]	1.09	1.11
2:B:1203:LYS:CD	2:B:1622:LYS:CB[5_445]	1.10	1.10
2:B:1203:LYS:O	2:B:1622:LYS:NZ[5_445]	1.13	1.07
2:B:1203:LYS:CB	2:B:1622:LYS:CD[5_445]	1.17	1.03
2:B:1203:LYS:CE	2:B:1622:LYS:C[5_445]	1.18	1.02
2:B:1105:GLN:N	2:B:1508:GLU:OE2[5_445]	1.22	0.98
2:B:1104:HIS:N	2:B:1508:GLU:CG[5_445]	1.24	0.96
2:B:1117:LYS:NZ	2:B:1632:GLU:OE1[5_445]	1.26	0.94
2:B:1203:LYS:CB	2:B:1622:LYS:CG[5_445]	1.29	0.91
2:B:1103:ILE:CG2	2:B:1512:ASP:OD2[5_445]	1.30	0.90
2:B:1103:ILE:O	2:B:1508:GLU:CB[5_445]	1.33	0.87
2:B:1114:ASN:OD1	2:B:1632:GLU:OE2[5_445]	1.34	0.86
2:B:1203:LYS:CE	2:B:1622:LYS:O[5_445]	1.35	0.85
2:B:1112:ARG:NH1	2:B:1507:LEU:N[5_445]	1.38	0.82
2:B:1203:LYS:CA	2:B:1622:LYS:NZ[5_445]	1.41	0.79
2:B:1105:GLN:CA	2:B:1508:GLU:OE2[5_445]	1.41	0.79
2:B:1203:LYS:NZ	2:B:1622:LYS:CA[5_445]	1.45	0.75
2:B:1114:ASN:OD1	2:B:1632:GLU:CB[5_445]	1.49	0.71
2:B:1202:GLY:O	2:B:1621:GLN:NE2[5_445]	1.50	0.70
2:B:1202:GLY:N	2:B:1621:GLN:CG[5_445]	1.51	0.69
2:B:1203:LYS:CE	2:B:1622:LYS:CA[5_445]	1.51	0.69
2:B:1112:ARG:O	2:B:1629:ALA:CB[5_445]	1.53	0.67
2:B:1203:LYS:CG	2:B:1622:LYS:CA[5_445]	1.54	0.66
2:B:1202:GLY:CA	2:B:1621:GLN:CD[5_445]	1.54	0.66
2:B:1098:GLU:O	2:B:1637:PHE:CZ[5_445]	1.55	0.65
2:B:1106:GLU:CB	2:B:1506:THR:CG2[5_445]	1.56	0.64
2:B:1103:ILE:CG2	2:B:1512:ASP:CG[5_445]	1.57	0.63
2:B:1104:HIS:C	2:B:1508:GLU:CG[5_445]	1.58	0.62
2:B:1103:ILE:O	2:B:1508:GLU:CA[5_445]	1.59	0.61
2:B:1203:LYS:C	2:B:1622:LYS:CE[5_445]	1.62	0.58
2:B:1104:HIS:C	2:B:1508:GLU:OE1[5_445]	1.63	0.57
2:B:1203:LYS:NZ	2:B:1622:LYS:O[5_445]	1.64	0.56
2:B:1203:LYS:CA	2:B:1622:LYS:CE[5_445]	1.65	0.55
2:B:1103:ILE:CG2	2:B:1512:ASP:OD1[5_445]	1.66	0.54
2:B:1202:GLY:C	2:B:1621:GLN:CB[5_445]	1.70	0.50
2:B:1114:ASN:OD1	2:B:1632:GLU:CD[5_445]	1.70	0.50
2:B:1203:LYS:CD	2:B:1622:LYS:CA[5_445]	1.71	0.49
2:B:1114:ASN:O	2:B:1632:GLU:OE2[5_445]	1.72	0.48
2:B:1202:GLY:N	2:B:1621:GLN:OE1[5_445]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:GLU:CD	2:B:1506:THR:CB[5_445]	1.79	0.41
2:B:1105:GLN:CA	2:B:1508:GLU:CD[5_445]	1.81	0.39
2:B:1114:ASN:CB	2:B:1628:GLY:O[5_445]	1.81	0.39
2:B:1114:ASN:OD1	2:B:1632:GLU:CG[5_445]	1.82	0.38
2:B:1203:LYS:CB	2:B:1622:LYS:CE[5_445]	1.82	0.38
2:B:1202:GLY:C	2:B:1621:GLN:NE2[5_445]	1.83	0.37
2:B:1202:GLY:N	2:B:1621:GLN:NE2[5_445]	1.84	0.36
2:B:1202:GLY:C	2:B:1621:GLN:CG[5_445]	1.86	0.34
2:B:1105:GLN:CA	2:B:1508:GLU:OE1[5_445]	1.86	0.34
2:B:1106:GLU:OE1	2:B:1507:LEU:N[5_445]	1.86	0.34
2:B:1103:ILE:C	2:B:1508:GLU:CG[5_445]	1.87	0.33
2:B:1105:GLN:N	2:B:1508:GLU:CG[5_445]	1.89	0.31
2:B:1104:HIS:CA	2:B:1508:GLU:CB[5_445]	1.90	0.30
2:B:1104:HIS:C	2:B:1508:GLU:OE2[5_445]	1.90	0.30
2:B:1103:ILE:C	2:B:1508:GLU:CB[5_445]	1.90	0.30
2:B:1202:GLY:C	2:B:1621:GLN:CD[5_445]	1.90	0.30
2:B:1244:TYR:OH	2:B:1509:GLU:CD[5_445]	1.91	0.29
2:B:1244:TYR:CE2	2:B:1506:THR:OG1[5_445]	1.92	0.28
2:B:1114:ASN:ND2	2:B:1632:GLU:N[5_445]	1.92	0.28
2:B:1204:GLN:N	2:B:1622:LYS:NZ[5_445]	1.94	0.26
2:B:1202:GLY:CA	2:B:1621:GLN:NE2[5_445]	1.95	0.25
2:B:1204:GLN:N	2:B:1622:LYS:CE[5_445]	1.98	0.22
2:B:1106:GLU:CG	2:B:1506:THR:CG2[5_445]	1.98	0.22
2:B:1203:LYS:CB	2:B:1622:LYS:NZ[5_445]	1.99	0.21
2:B:1106:GLU:OE2	2:B:1506:THR:CB[5_445]	1.99	0.21
2:B:1112:ARG:NH1	2:B:1506:THR:C[5_445]	1.99	0.21
2:B:1114:ASN:CG	2:B:1632:GLU:CB[5_445]	2.00	0.20
2:B:1112:ARG:CZ	2:B:1507:LEU:N[5_445]	2.01	0.19
2:B:1200:ASP:O	2:B:1621:GLN:OE1[5_445]	2.05	0.15
2:B:1244:TYR:OH	2:B:1509:GLU:OE2[5_445]	2.06	0.14
2:B:1104:HIS:CA	2:B:1508:GLU:CD[5_445]	2.08	0.12
2:B:1106:GLU:N	2:B:1508:GLU:OE1[5_445]	2.09	0.11
2:B:1203:LYS:CA	2:B:1622:LYS:CG[5_445]	2.09	0.11
2:B:1117:LYS:NZ	2:B:1632:GLU:CD[5_445]	2.09	0.11
2:B:1103:ILE:CG1	2:B:1512:ASP:OD1[5_445]	2.10	0.10
2:B:1163:ARG:NH2	2:B:1625:GLN:NE2[5_445]	2.10	0.10
2:B:1104:HIS:N	2:B:1508:GLU:CB[5_445]	2.12	0.08
2:B:1114:ASN:ND2	2:B:1632:GLU:CB[5_445]	2.12	0.08
2:B:1114:ASN:CG	2:B:1632:GLU:OE2[5_445]	2.13	0.07
2:B:1203:LYS:CE	2:B:1622:LYS:CB[5_445]	2.13	0.07
2:B:1104:HIS:O	2:B:1508:GLU:CD[5_445]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1203:LYS:CG	2:B:1622:LYS:N[5_445]	2.14	0.06
2:B:1106:GLU:OE2	2:B:1509:GLU:CG[5_445]	2.15	0.05
2:B:1103:ILE:CB	2:B:1512:ASP:OD1[5_445]	2.15	0.05
2:B:1105:GLN:C	2:B:1508:GLU:OE1[5_445]	2.18	0.02
2:B:1112:ARG:CZ	2:B:1507:LEU:CA[5_445]	2.18	0.02
2:B:1203:LYS:CA	2:B:1622:LYS:CD[5_445]	2.18	0.02
2:B:1103:ILE:O	2:B:1508:GLU:C[5_445]	2.19	0.01
2:B:1203:LYS:CG	2:B:1622:LYS:CD[5_445]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	640/642 (100%)	526 (82%)	93 (14%)	21 (3%)	5 43
2	B	897/915 (98%)	748 (83%)	112 (12%)	37 (4%)	3 36
3	S	117/119 (98%)	99 (85%)	15 (13%)	3 (3%)	7 48
All	All	1654/1676 (99%)	1373 (83%)	220 (13%)	61 (4%)	4 40

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	198	THR
1	A	294	ALA
1	A	549	GLU
1	A	552	GLN
2	B	733	ILE
2	B	928	GLU
2	B	1238	ARG
2	B	1247	THR
2	B	1378	MET
2	B	1429	VAL

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Mol	Chain	Res	Type
2	B	1450	ILE
2	B	1465	GLU
2	B	1498	ILE
2	B	1602	LYS
1	A	40	PHE
1	A	292	LEU
1	A	293	ARG
1	A	548	SER
1	A	551	ARG
2	B	869	LYS
2	B	932	ARG
2	B	1038	ARG
2	B	1106	GLU
2	B	1292	GLU
2	B	1334	LEU
2	B	1375	ASP
2	B	1478	GLY
2	B	1517	PRO
2	B	1619	GLU
3	S	103	GLY
1	A	132	HIS
1	A	393	PRO
1	A	442	GLU
2	B	967	GLN
2	B	1013	GLU
2	B	1196	ASN
2	B	1486	ASP
2	B	1551	SER
2	B	1573	LYS
2	B	1583	TRP
3	S	64	GLN
1	A	70	ALA
1	A	408	GLU
1	A	607	PRO
2	B	911	PRO
2	B	944	ASP
2	B	988	CYS
2	B	1576	GLU
1	A	50	GLU
1	A	364	ARG
2	B	778	THR
2	B	1314	GLY

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Mol	Chain	Res	Type
2	B	1315	LYS
1	A	148	PRO
1	A	219	LYS
1	A	238	LEU
2	B	1349	PRO
3	S	20	LEU
2	B	1145	GLY
2	B	913	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	566/566 (100%)	491 (87%)	75 (13%)	5 30
2	B	799/810 (99%)	723 (90%)	76 (10%)	11 45
3	S	109/109 (100%)	96 (88%)	13 (12%)	6 35
All	All	1474/1485 (99%)	1310 (89%)	164 (11%)	8 38

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	8	THR
1	A	10	ASN
1	A	13	ARG
1	A	20	MET
1	A	44	LYS
1	A	45	LEU
1	A	47	LEU
1	A	51	LYS
1	A	71	ASN
1	A	74	PHE
1	A	112	THR
1	A	118	THR
1	A	125	TYR

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Mol	Chain	Res	Type
1	A	140	THR
1	A	142	MET
1	A	156	ASP
1	A	158	LEU
1	A	159	SER
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	179	MET
1	A	183	LYS
1	A	207	LEU
1	A	209	SER
1	A	212	VAL
1	A	215	GLU
1	A	230	GLU
1	A	249	VAL
1	A	258	GLN
1	A	285	LEU
1	A	295	GLU
1	A	301	SER
1	A	321	ARG
1	A	322	SER
1	A	328	THR
1	A	336	THR
1	A	350	LEU
1	A	373	ASP
1	A	377	SER
1	A	379	THR
1	A	389	ILE
1	A	399	SER
1	A	404	THR
1	A	409	LEU
1	A	416	THR
1	A	426	THR
1	A	443	LEU
1	A	448	THR
1	A	452	ASN
1	A	462	GLU
1	A	464	LYS
1	A	471	LEU
1	A	474	ASN
1	A	477	ARG

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Mol	Chain	Res	Type
1	A	494	VAL
1	A	498	SER
1	A	500	THR
1	A	509	LEU
1	A	514	THR
1	A	515	LEU
1	A	521	GLN
1	A	528	SER
1	A	535	ASP
1	A	537	CYS
1	A	540	SER
1	A	542	VAL
1	A	551	ARG
1	A	554	VAL
1	A	587	ASN
1	A	611	LYS
1	A	618	SER
1	A	625	THR
1	A	639	GLN
2	B	748	SER
2	B	752	ASN
2	B	758	GLU
2	B	766	THR
2	B	789	ASP
2	B	802	THR
2	B	825	ILE
2	B	835	ASN
2	B	836	GLN
2	B	841	ARG
2	B	863	THR
2	B	917	ASN
2	B	922	VAL
2	B	939	ASP
2	B	953	GLU
2	B	957	ARG
2	B	959	LEU
2	B	963	THR
2	B	968	MET
2	B	974	ASP
2	B	984	THR
2	B	994	ILE
2	B	1018	GLU

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Mol	Chain	Res	Type
2	B	1066	LEU
2	B	1069	ASN
2	B	1076	GLN
2	B	1136	CYS
2	B	1137	GLU
2	B	1138	GLU
2	B	1255	GLN
2	B	1259	GLN
2	B	1266	ASP
2	B	1288	ARG
2	B	1295	SER
2	B	1302	THR
2	B	1313	GLU
2	B	1320	LEU
2	B	1321	SER
2	B	1337	ASN
2	B	1339	PHE
2	B	1344	THR
2	B	1360	ASN
2	B	1361	THR
2	B	1369	ARG
2	B	1374	GLN
2	B	1387	THR
2	B	1393	THR
2	B	1403	VAL
2	B	1408	SER
2	B	1418	ASP
2	B	1422	LEU
2	B	1428	LYS
2	B	1432	SER
2	B	1445	PHE
2	B	1457	VAL
2	B	1462	ASN
2	B	1487	GLU
2	B	1504	LYS
2	B	1505	VAL
2	B	1506	THR
2	B	1507	LEU
2	B	1529	LYS
2	B	1564	SER
2	B	1566	ILE
2	B	1567	LYS

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Mol	Chain	Res	Type
2	B	1573	LYS
2	B	1577	LYS
2	B	1578	LYS
2	B	1583	TRP
2	B	1590	TRP
2	B	1593	LYS
2	B	1597	SER
2	B	1604	THR
2	B	1606	VAL
2	B	1624	CYS
2	B	1631	THR
3	S	1	ARG
3	S	3	ILE
3	S	23	THR
3	S	31	THR
3	S	50	LEU
3	S	56	ASP
3	S	66	ARG
3	S	81	LEU
3	S	85	GLU
3	S	87	ASP
3	S	90	SER
3	S	95	GLU
3	S	109	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	38	HIS
1	A	71	ASN
1	A	81	ASN
1	A	93	GLN
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	162	ASN
1	A	193	GLN
1	A	376	GLN
1	A	420	GLN
1	A	452	ASN
1	A	490	GLN

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Mol	Chain	Res	Type
1	A	521	GLN
2	B	834	GLN
2	B	835	ASN
2	B	836	GLN
2	B	897	HIS
2	B	961	GLN
2	B	1004	HIS
2	B	1033	GLN
2	B	1069	ASN
2	B	1105	GLN
2	B	1114	ASN
2	B	1141	ASN
2	B	1160	ASN
2	B	1204	GLN
2	B	1235	ASN
2	B	1271	ASN
2	B	1277	GLN
2	B	1290	HIS
2	B	1360	ASN
2	B	1401	ASN
2	B	1462	ASN
3	S	40	GLN

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)

4 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	$\#\|Z\|>2$
4	NAG	A	643	1,4	14,14,15	0.77	0	15,19,21	1.56	2 (13%)
4	NAG	A	644	4	14,14,15	0.44	0	15,19,21	2.15	3 (20%)
4	BMA	A	645	4	11,11,12	0.69	0	14,15,17	1.50	2 (14%)
4	BMA	A	646	4	11,11,12	0.57	0	14,15,17	0.76	1 (7%)

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
4	NAG	A	643	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	644	4	-	0/6/23/26	0/1/1/1
4	BMA	A	645	4	-	0/2/19/22	0/1/1/1
4	BMA	A	646	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	643	NAG	C1-O5-C5	-3.58	107.70	112.25
4	A	644	NAG	C4-C3-C2	-2.50	107.34	111.23
4	A	646	BMA	O5-C1-C2	-2.12	107.42	110.86
4	A	645	BMA	C1-C2-C3	2.23	112.18	109.54
4	A	644	NAG	O4-C4-C5	2.84	116.75	109.24
4	A	643	NAG	C4-C3-C2	3.52	116.71	111.23
4	A	645	BMA	C1-O5-C5	4.56	118.04	112.25
4	A	644	NAG	C1-O5-C5	6.69	120.74	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	643	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	B	5	2	14,14,15	0.59	0	15,19,21	1.35	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
5	NAG	B	5	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5	NAG	C1-O5-C5	3.35	116.50	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	642/642 (100%)	-0.57	0 100 100	147, 191, 237, 314	0
2	B	761/915 (83%)	-0.31	13 (1%) 73 63	135, 206, 258, 294	0
3	S	119/119 (100%)	-0.30	3 (2%) 61 49	167, 203, 249, 289	0
All	All	1522/1676 (90%)	-0.42	16 (1%) 82 75	135, 199, 249, 314	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1244	TYR	4.5
2	B	1114	ASN	4.0
2	B	1113	ASN	3.5
2	B	1137	GLU	3.2
2	B	1115	ASN	2.9
3	S	42	GLY	2.8
3	S	118	LYS	2.6
2	B	1093	ASP	2.5
3	S	0	GLY	2.4
2	B	1162	GLN	2.4
2	B	1240	TYR	2.2
2	B	1182	GLY	2.2
2	B	1094	GLY	2.1
2	B	1099	ASP	2.1
2	B	887	GLU	2.0
2	B	1483	LEU	2.0

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 (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
4	NAG	A	643	14/15	0.92	0.20	-0.16	207,210,212,214	0
4	BMA	A	645	11/12	0.85	0.47	-	233,236,238,238	0
4	NAG	A	644	14/15	0.87	0.41	-	215,220,226,233	0
4	BMA	A	646	11/12	0.78	0.36	-	222,223,226,228	11

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	NAG	B	5	14/15	0.92	0.22	0.21	232,236,237,238	0
6	CA	A	647	1/1	0.96	0.08	-3.34	123,123,123,123	0

6.5 Other polymers (i)

There are no such residues in this entry.