Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:09 PM GMT

PDB ID	:	4UY2
Title	:	Crystal structure of the complex of the extracellular domain of human alpha9 nAChR with alpha-bungarotoxin.
Authors	:	Giastas, P.; Zouridakis, M.; Zarkadas, E.; Tzartos, S.J.
Deposited on	:	2014-08-28
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

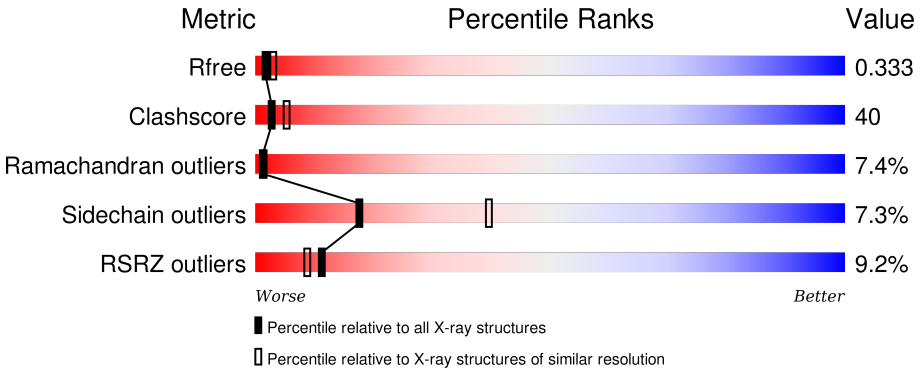
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	218	9% 47% 39% 5% • 7%
1	B	218	10% 46% 36% 8% • 7%
2	C	74	8% 43% 38% 15% • •
2	D	74	5% 47% 35% 14% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4468 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 NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1658	1061	270	321	6			
1	B	203	Total	C	N	O	S	0	0	0
			1658	1061	270	321	6			

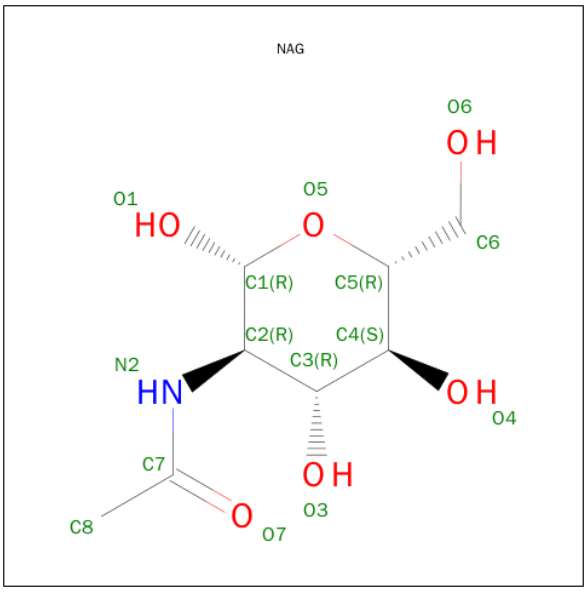
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	HIS	-	EXPRESSION TAG	UNP Q9UGM1
A	214	HIS	-	EXPRESSION TAG	UNP Q9UGM1
A	215	HIS	-	EXPRESSION TAG	UNP Q9UGM1
A	216	HIS	-	EXPRESSION TAG	UNP Q9UGM1
A	217	HIS	-	EXPRESSION TAG	UNP Q9UGM1
A	218	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	213	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	214	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	215	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	216	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	217	HIS	-	EXPRESSION TAG	UNP Q9UGM1
B	218	HIS	-	EXPRESSION TAG	UNP Q9UGM1

- Molecule 2 is a protein called ALPHA-BUNGAROTOXIN ISOFORM V31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	73	Total	C	N	O	S	0	0	0
			548	338	96	103	11			
2	D	73	Total	C	N	O	S	0	0	0
			548	338	96	103	11			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



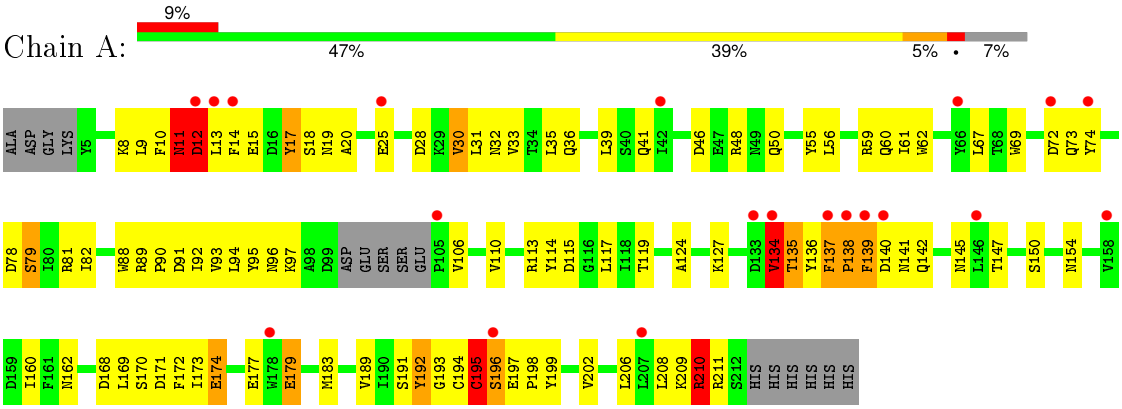
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

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.

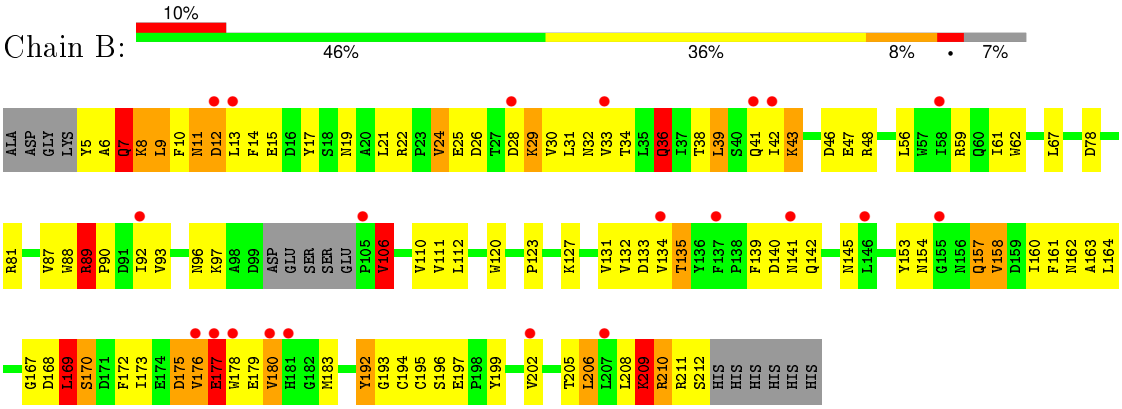
• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-9

Chain A:



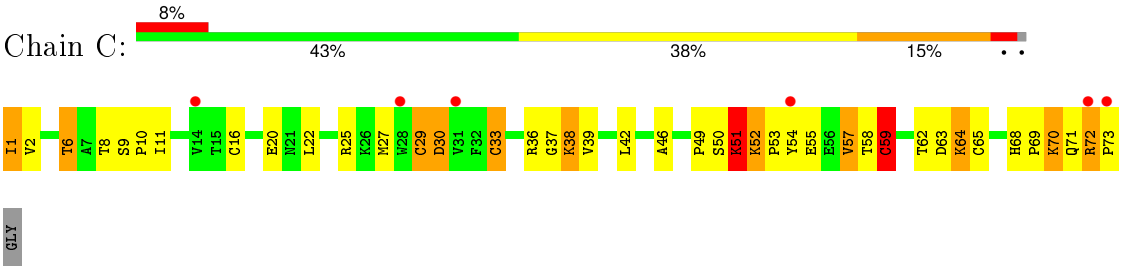
• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-9

Chain B:



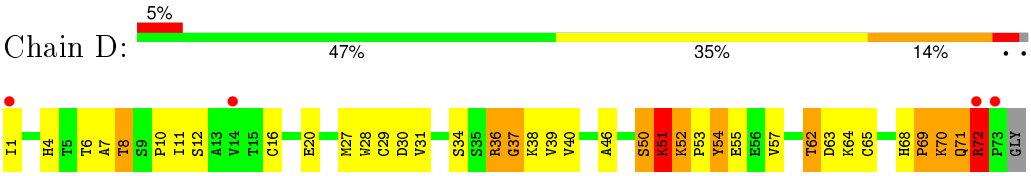
• Molecule 2: ALPHA-BUNGAROTOXIN ISOFORM V31

Chain C:



• Molecule 2: ALPHA-BUNGAROTOXIN ISOFORM V31

Chain D:


5%
47%
35%
14%
I1
H4
T5
T6
A7
T8
S9
P10
I11
S12
A13
V14
T15
C16
E20
M27
W28
C29
D30
V31
S34
S35
R36
G37
K38
V39
V40
A46
S50
K51
K52
P53
Y54
E55
E56
V57
T62
D63
K64
C65
H68
P69
K70
Q71
R72
P73
G1Y

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.32Å 119.35Å 79.11Å 90.00° 103.02° 90.00°	Depositor
Resolution (Å)	47.19 – 2.70 47.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.19-2.70) 99.5 (47.18-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.258 , 0.331 0.257 , 0.333	Depositor DCC
R_{free} test set	1037 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 90.5	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 21021 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.59 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3104e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.75	0/1700	1.13	8/2323 (0.3%)
1	B	0.75	1/1700 (0.1%)	1.13	13/2323 (0.6%)
2	C	0.90	3/562 (0.5%)	1.17	4/765 (0.5%)
2	D	0.84	0/562	1.29	5/765 (0.7%)
All	All	0.78	4/4524 (0.1%)	1.16	30/6176 (0.5%)

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	4
1	B	0	6
2	C	0	3
2	D	0	2
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	51	LYS	CG-CD	-5.63	1.33	1.52
2	C	57	VAL	CB-CG1	5.63	1.64	1.52
1	B	180	VAL	CB-CG1	5.31	1.64	1.52
2	C	57	VAL	CA-CB	-5.18	1.43	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ARG	NE-CZ-NH1	11.18	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	ARG	NE-CZ-NH1	10.54	125.57	120.30
2	D	51	LYS	CD-CE-NZ	10.50	135.85	111.70
1	A	137	PHE	C-N-CD	-9.54	99.61	120.60
1	B	164	LEU	CA-CB-CG	8.81	135.55	115.30
2	D	72	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	B	177	GLU	N-CA-C	7.68	131.75	111.00
2	C	57	VAL	CG1-CB-CG2	7.60	123.06	110.90
1	A	127	LYS	CD-CE-NZ	7.38	128.66	111.70
1	A	12	ASP	N-CA-C	7.02	129.95	111.00
1	B	36	GLN	CA-CB-CG	6.25	127.16	113.40
1	B	209	LYS	CD-CE-NZ	6.12	125.78	111.70
1	B	89	ARG	CD-NE-CZ	6.07	132.10	123.60
1	A	12	ASP	CA-C-N	-6.01	103.98	117.20
2	C	57	VAL	CA-CB-CG2	-5.91	102.03	110.90
1	B	56	LEU	CA-CB-CG	5.69	128.39	115.30
2	D	71	GLN	CA-CB-CG	5.61	125.74	113.40
1	A	210	ARG	CD-NE-CZ	5.47	131.25	123.60
1	B	206	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	A	12	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	175	ASP	CB-CG-OD1	5.39	123.15	118.30
2	C	51	LYS	N-CA-C	5.39	125.54	111.00
2	C	59	CYS	CA-CB-SG	5.33	123.60	114.00
1	B	177	GLU	CB-CA-C	-5.29	99.82	110.40
1	B	39	LEU	CB-CG-CD2	-5.27	102.05	111.00
2	D	51	LYS	CG-CD-CE	-5.23	96.22	111.90
2	D	36	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	B	169	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	196	SER	N-CA-CB	5.08	118.11	110.50
1	B	177	GLU	CA-C-N	-5.01	106.18	117.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASN	Peptide
1	A	134	VAL	Peptide
1	A	135	THR	Peptide
1	A	195	CYS	Peptide
1	B	12	ASP	Peptide
1	B	176	VAL	Peptide
1	B	177	GLU	Peptide
1	B	195	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	7	GLN	Peptide
1	B	9	LEU	Peptide
2	C	29	CYS	Peptide
2	C	51	LYS	Peptide
2	C	64	LYS	Peptide
2	D	52	LYS	Peptide
2	D	72	ARG	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	1658	0	1577	118	0
1	B	1658	0	1577	149	0
2	C	548	0	533	51	0
2	D	548	0	533	52	0
3	A	28	0	26	1	0
3	B	28	0	26	2	0
All	All	4468	0	4272	352	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 40.

All (352) 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:142:GLN:H	1:B:209:LYS:HE3	1.17	1.04
1:A:210:ARG:HD3	1:A:211:ARG:N	1.77	0.99
1:A:177:GLU:HA	1:A:210:ARG:HE	1.28	0.97
1:A:179:GLU:OE2	1:A:210:ARG:NH2	1.96	0.96
1:A:210:ARG:HH11	1:A:211:ARG:H	1.07	0.95
1:B:62:TRP:HZ2	1:B:89:ARG:HD2	1.31	0.95
1:A:209:LYS:HD2	1:A:210:ARG:H	1.32	0.94
2:D:51:LYS:HE2	2:D:55:GLU:HB2	1.48	0.94
2:C:72:ARG:HG3	2:C:73:PRO:HD2	1.47	0.93
1:A:210:ARG:NH1	1:A:211:ARG:H	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:ND2	1:A:145:ASN:O	2.00	0.93
1:A:210:ARG:HA	1:A:210:ARG:HH11	1.34	0.91
2:C:49:PRO:O	2:C:51:LYS:NZ	2.07	0.88
1:B:142:GLN:N	1:B:209:LYS:HE3	1.88	0.87
1:B:8:LYS:HG3	1:B:11:ASN:HA	1.56	0.87
1:B:7:GLN:HE21	1:B:9:LEU:H	1.19	0.86
1:A:134:VAL:HG13	1:A:137:PHE:HE1	1.42	0.84
1:A:210:ARG:HA	1:A:210:ARG:NH1	1.93	0.83
1:B:142:GLN:H	1:B:209:LYS:CE	1.90	0.83
1:B:62:TRP:CZ2	1:B:89:ARG:HD2	2.15	0.82
1:B:193:GLY:N	2:D:38:LYS:O	2.12	0.81
1:A:209:LYS:CD	1:A:210:ARG:H	1.93	0.81
1:A:210:ARG:CZ	1:A:211:ARG:HG2	2.11	0.80
1:A:210:ARG:HH11	1:A:211:ARG:N	1.78	0.80
1:B:141:ASN:HA	1:B:209:LYS:HE3	1.62	0.79
2:D:51:LYS:HD2	2:D:57:VAL:HB	1.63	0.79
1:A:17:TYR:OH	1:A:88:TRP:N	2.14	0.79
1:B:87:VAL:HB	1:B:89:ARG:HE	1.47	0.77
1:A:177:GLU:CA	1:A:210:ARG:HE	1.97	0.77
1:B:96:ASN:ND2	1:B:145:ASN:O	2.18	0.77
1:B:133:ASP:N	1:B:141:ASN:O	2.18	0.77
1:A:41:GLN:HB2	1:B:173:ILE:HD13	1.67	0.77
2:D:51:LYS:HE2	2:D:55:GLU:CB	2.14	0.76
1:B:154:ASN:OD1	1:B:157:GLN:HG2	1.85	0.76
2:D:51:LYS:NZ	2:D:57:VAL:HG23	2.00	0.76
1:B:81:ARG:HD3	1:B:111:VAL:HG22	1.67	0.76
2:C:51:LYS:CD	2:C:57:VAL:HG21	2.16	0.76
2:D:70:LYS:HG3	2:D:71:GLN:H	1.50	0.75
2:C:51:LYS:NZ	2:C:57:VAL:HG11	2.01	0.75
2:C:55:GLU:HB3	2:C:57:VAL:HG23	1.67	0.74
1:A:10:PHE:O	1:A:12:ASP:HB3	1.87	0.74
1:A:59:ARG:HH12	1:A:119:THR:HG23	1.52	0.74
2:D:51:LYS:HZ2	2:D:57:VAL:H	1.36	0.73
1:A:10:PHE:C	1:A:12:ASP:HB3	2.10	0.72
1:A:138:PRO:HB2	1:A:209:LYS:HG2	1.71	0.72
2:D:51:LYS:HZ2	2:D:57:VAL:N	1.87	0.72
1:B:9:LEU:C	1:B:11:ASN:H	1.93	0.72
1:A:90:PRO:O	1:A:92:ILE:N	2.24	0.71
2:C:72:ARG:HG3	2:C:73:PRO:CD	2.21	0.71
1:B:8:LYS:HE3	1:B:11:ASN:O	1.92	0.70
1:B:175:ASP:OD1	1:B:177:GLU:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:LYS:NZ	2:D:57:VAL:H	1.89	0.70
2:C:1:ILE:HD12	2:C:2:VAL:N	2.07	0.70
2:C:50:SER:O	2:C:51:LYS:HE2	1.92	0.69
1:A:8:LYS:HD2	1:A:11:ASN:HB3	1.74	0.69
2:C:51:LYS:HZ1	2:C:57:VAL:HG11	1.54	0.69
2:C:51:LYS:HG3	2:C:52:LYS:HG2	1.75	0.69
2:C:51:LYS:HD2	2:C:57:VAL:HG21	1.74	0.69
1:A:95:TYR:OH	2:C:36:ARG:NH2	2.25	0.69
2:D:51:LYS:HZ2	2:D:57:VAL:HG23	1.57	0.69
1:A:189:VAL:HB	1:A:198:PRO:HB2	1.75	0.69
1:A:209:LYS:HD2	1:A:210:ARG:N	2.06	0.68
1:A:25:GLU:N	1:A:25:GLU:OE1	2.26	0.68
2:D:69:PRO:C	2:D:72:ARG:HH12	1.97	0.67
1:B:7:GLN:NE2	1:B:9:LEU:H	1.92	0.67
1:A:139:PHE:HB3	1:A:209:LYS:NZ	2.11	0.66
1:A:194:CYS:HB3	2:C:37:GLY:N	2.11	0.66
1:B:175:ASP:O	1:B:177:GLU:HG3	1.95	0.66
2:D:38:LYS:HE3	2:D:54:TYR:CE1	2.31	0.66
2:D:4:HIS:NE2	2:D:64:LYS:HE3	2.11	0.66
1:B:36:GLN:HA	1:B:36:GLN:HE21	1.61	0.66
1:B:208:LEU:O	1:B:209:LYS:HG2	1.95	0.66
1:A:134:VAL:HG13	1:A:137:PHE:CE1	2.29	0.66
1:B:88:TRP:O	1:B:89:ARG:CZ	2.45	0.65
1:A:79:SER:HB2	1:A:113:ARG:HA	1.79	0.65
2:D:8:THR:HG21	2:D:12:SER:OG	1.97	0.65
1:A:169:LEU:O	1:A:172:PHE:N	2.31	0.64
1:B:62:TRP:HE1	1:B:89:ARG:NH1	1.95	0.64
1:B:194:CYS:HB3	2:D:36:ARG:C	2.18	0.64
1:B:39:LEU:HD21	1:B:172:PHE:HD1	1.62	0.64
1:B:62:TRP:CZ2	1:B:89:ARG:CD	2.81	0.64
1:B:6:ALA:O	1:B:7:GLN:NE2	2.30	0.63
1:A:195:CYS:HB2	1:A:196:SER:OG	1.97	0.63
1:A:59:ARG:HH12	1:A:119:THR:CG2	2.12	0.63
1:A:135:THR:O	1:A:136:TYR:CD2	2.51	0.63
2:C:1:ILE:HD12	2:C:2:VAL:H	1.64	0.62
1:A:139:PHE:HB3	1:A:209:LYS:HZ1	1.63	0.62
1:A:206:LEU:HG	1:A:208:LEU:HD21	1.82	0.62
1:B:24:VAL:HG11	1:B:29:LYS:HB2	1.81	0.62
1:B:47:GLU:OE2	1:B:210:ARG:NH2	2.32	0.62
2:D:51:LYS:CE	2:D:55:GLU:HB2	2.26	0.62
1:B:31:LEU:HD21	1:B:62:TRP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HG3	1:B:11:ASN:CA	2.30	0.62
1:B:38:THR:HG23	1:B:168:ASP:HB3	1.80	0.62
1:B:169:LEU:O	1:B:172:PHE:N	2.33	0.62
1:A:210:ARG:HD3	1:A:210:ARG:C	2.18	0.61
1:B:140:ASP:OD2	1:B:210:ARG:NE	2.33	0.61
1:B:59:ARG:HD3	1:B:61:ILE:HD11	1.82	0.61
1:B:39:LEU:HD21	1:B:172:PHE:CD1	2.35	0.61
1:B:177:GLU:OE1	1:B:179:GLU:HB3	2.01	0.61
1:A:162:ASN:N	1:A:162:ASN:OD1	2.33	0.61
1:B:192:TYR:H	2:D:39:VAL:HG13	1.65	0.61
2:D:68:HIS:C	2:D:70:LYS:H	2.03	0.61
1:A:33:VAL:HG22	1:A:62:TRP:HB3	1.82	0.61
1:B:133:ASP:OD1	1:B:135:THR:HB	2.02	0.60
1:A:30:VAL:O	3:A:1214:NAG:H82	2.00	0.60
1:B:140:ASP:C	1:B:141:ASN:HD22	2.05	0.60
1:A:36:GLN:NE2	1:A:168:ASP:HB2	2.17	0.60
1:B:179:GLU:OE2	1:B:210:ARG:N	2.35	0.59
2:C:51:LYS:HD2	2:C:55:GLU:HG3	1.84	0.59
2:C:8:THR:HG23	2:C:10:PRO:O	2.02	0.59
1:A:9:LEU:HA	1:A:74:TYR:HE2	1.67	0.59
1:A:134:VAL:HG21	1:A:140:ASP:HA	1.83	0.59
1:B:133:ASP:OD1	1:B:135:THR:N	2.35	0.59
1:B:87:VAL:CB	1:B:89:ARG:HE	2.16	0.59
1:B:22:ARG:HG2	1:B:88:TRP:CZ2	2.38	0.59
1:B:12:ASP:CG	1:B:15:GLU:HB2	2.22	0.59
1:A:17:TYR:CD2	1:A:67:LEU:HD21	2.37	0.59
2:C:29:CYS:HB2	2:C:54:TYR:HE2	1.68	0.59
1:A:138:PRO:CB	1:A:209:LYS:HG2	2.32	0.59
1:A:35:LEU:HD12	1:A:60:GLN:HG2	1.85	0.58
1:B:88:TRP:O	1:B:89:ARG:NH1	2.37	0.58
1:B:140:ASP:H	1:B:141:ASN:ND2	2.02	0.57
2:C:20:GLU:HA	2:C:46:ALA:HA	1.85	0.57
2:C:25:ARG:O	2:C:57:VAL:HA	2.03	0.57
1:B:7:GLN:HE21	1:B:9:LEU:N	1.95	0.57
1:B:88:TRP:HE3	1:B:89:ARG:NH1	2.02	0.57
2:C:42:LEU:HD11	2:C:68:HIS:HB2	1.87	0.57
1:B:177:GLU:HB2	1:B:211:ARG:HE	1.69	0.57
1:A:177:GLU:HA	1:A:210:ARG:NE	2.10	0.57
1:A:169:LEU:O	1:A:171:ASP:N	2.38	0.57
2:C:30:ASP:OD1	2:C:33:CYS:N	2.38	0.57
1:A:173:ILE:HD13	1:B:41:GLN:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:HB2	1:A:14:PHE:HD2	1.70	0.57
1:B:153:TYR:HB3	1:B:158:VAL:HG13	1.86	0.56
1:B:88:TRP:O	1:B:88:TRP:CE3	2.58	0.56
1:B:180:VAL:HG22	1:B:206:LEU:HD11	1.86	0.56
1:B:141:ASN:HA	1:B:209:LYS:CE	2.34	0.56
2:C:6:THR:HA	2:C:11:ILE:CD1	2.35	0.56
2:D:53:PRO:HD2	2:D:55:GLU:HG3	1.88	0.56
1:B:87:VAL:HB	1:B:89:ARG:NE	2.19	0.56
1:B:194:CYS:HB3	2:D:37:GLY:N	2.20	0.56
2:C:29:CYS:HB2	2:C:54:TYR:CE2	2.40	0.56
2:C:63:ASP:O	2:C:64:LYS:HB2	2.06	0.56
1:B:106:VAL:CG1	1:B:123:PRO:HG2	2.35	0.56
1:B:178:TRP:HA	1:B:179:GLU:OE2	2.07	0.55
1:A:31:LEU:HD21	1:A:62:TRP:HB2	1.87	0.55
1:A:61:ILE:HG22	1:A:117:LEU:HD11	1.88	0.55
1:B:78:ASP:OD1	1:B:78:ASP:N	2.32	0.55
1:B:7:GLN:HG2	1:B:8:LYS:N	2.22	0.55
1:B:8:LYS:HD2	1:B:10:PHE:CD2	2.42	0.55
1:B:36:GLN:NE2	1:B:36:GLN:HA	2.21	0.55
1:B:62:TRP:HE1	1:B:89:ARG:CZ	2.20	0.55
1:B:141:ASN:CA	1:B:209:LYS:HE3	2.36	0.55
1:A:183:MET:HG3	1:A:206:LEU:HD13	1.90	0.54
1:A:56:LEU:O	1:A:124:ALA:N	2.39	0.54
1:A:72:ASP:OD1	1:A:73:GLN:N	2.40	0.54
1:A:72:ASP:OD1	1:A:73:GLN:HG3	2.06	0.54
1:B:34:THR:HG22	1:B:163:ALA:HB2	1.88	0.54
1:B:177:GLU:OE2	1:B:211:ARG:NH2	2.41	0.54
2:D:50:SER:O	2:D:51:LYS:HG2	2.08	0.54
2:D:27:MET:HG2	2:D:40:VAL:HG22	1.90	0.54
2:D:1:ILE:HG23	2:D:16:CYS:SG	2.48	0.54
1:B:87:VAL:O	1:B:89:ARG:HG2	2.07	0.53
1:B:177:GLU:CD	1:B:211:ARG:HH21	2.10	0.53
1:B:179:GLU:N	1:B:179:GLU:CD	2.62	0.53
1:A:134:VAL:CG2	1:A:141:ASN:H	2.22	0.53
1:B:88:TRP:HE3	1:B:89:ARG:HH11	1.56	0.53
2:D:4:HIS:CE1	2:D:64:LYS:HE3	2.42	0.53
1:A:10:PHE:O	1:A:10:PHE:CD1	2.61	0.53
1:B:13:LEU:O	1:B:17:TYR:HB2	2.08	0.53
1:B:208:LEU:H	1:B:209:LYS:HZ3	1.57	0.53
2:C:54:TYR:CG	2:C:54:TYR:O	2.60	0.53
1:A:9:LEU:HD11	1:A:13:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:LYS:HG3	2:C:52:LYS:CG	2.39	0.52
1:B:194:CYS:SG	2:D:36:ARG:HB2	2.50	0.52
1:B:141:ASN:HA	1:B:209:LYS:HD2	1.92	0.52
2:D:54:TYR:O	2:D:54:TYR:HD1	1.93	0.52
1:A:93:VAL:HG23	1:A:94:LEU:N	2.24	0.52
1:A:173:ILE:HD13	1:B:41:GLN:CB	2.40	0.52
2:C:72:ARG:CG	2:C:73:PRO:HD2	2.30	0.52
1:A:210:ARG:NE	1:A:211:ARG:HG2	2.25	0.52
1:A:28:ASP:N	1:A:28:ASP:OD1	2.36	0.52
2:D:20:GLU:HA	2:D:46:ALA:HA	1.91	0.51
1:B:11:ASN:CG	1:B:12:ASP:H	2.14	0.51
1:A:9:LEU:HB2	1:A:74:TYR:HD2	1.76	0.51
1:A:17:TYR:HD2	1:A:67:LEU:HD21	1.75	0.51
1:A:59:ARG:NH1	1:A:119:THR:HG23	2.23	0.51
1:B:11:ASN:OD1	1:B:13:LEU:HG	2.11	0.51
2:D:68:HIS:O	2:D:70:LYS:N	2.44	0.50
1:A:12:ASP:C	1:A:14:PHE:H	2.15	0.50
2:C:50:SER:C	2:C:51:LYS:HE2	2.31	0.50
1:A:177:GLU:O	1:A:210:ARG:HB2	2.11	0.50
2:C:51:LYS:HD3	2:C:57:VAL:HG21	1.90	0.50
1:B:25:GLU:HB2	1:B:29:LYS:NZ	2.27	0.50
1:B:41:GLN:OE1	1:B:42:ILE:N	2.44	0.50
1:B:5:TYR:HD2	1:B:6:ALA:H	1.55	0.50
1:B:179:GLU:OE2	1:B:209:LYS:N	2.35	0.49
1:B:106:VAL:HG11	1:B:123:PRO:HG2	1.94	0.49
2:D:1:ILE:HD12	2:D:63:ASP:OD1	2.12	0.49
1:A:137:PHE:HA	1:A:138:PRO:O	2.12	0.49
1:A:179:GLU:CD	1:A:210:ARG:HH22	2.15	0.49
2:D:71:GLN:O	2:D:72:ARG:HG2	2.12	0.49
1:B:177:GLU:HG2	1:B:178:TRP:O	2.12	0.49
1:B:208:LEU:C	1:B:209:LYS:HZ3	2.15	0.49
2:D:51:LYS:CE	2:D:57:VAL:H	2.25	0.49
2:C:51:LYS:HG3	2:C:55:GLU:HG3	1.94	0.49
2:D:68:HIS:C	2:D:70:LYS:N	2.66	0.49
1:B:141:ASN:HD22	1:B:141:ASN:N	2.09	0.49
2:D:6:THR:C	2:D:8:THR:H	2.15	0.49
1:B:183:MET:HG3	1:B:206:LEU:HD13	1.95	0.49
1:B:30:VAL:O	3:B:1214:NAG:H82	2.12	0.49
1:B:160:ILE:HD12	1:B:202:VAL:HG13	1.95	0.49
1:A:140:ASP:H	1:A:209:LYS:HD3	1.78	0.48
1:A:50:GLN:HE21	1:A:142:GLN:HE21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:C	1:B:177:GLU:HG3	2.32	0.48
1:B:167:GLY:HA3	1:B:183:MET:SD	2.53	0.48
2:C:52:LYS:HB2	2:C:55:GLU:CG	2.43	0.48
1:B:208:LEU:N	1:B:209:LYS:HZ3	2.11	0.48
2:C:70:LYS:CG	2:C:71:GLN:H	2.26	0.48
1:A:12:ASP:OD1	1:A:15:GLU:OE1	2.32	0.48
1:B:28:ASP:OD1	1:B:28:ASP:N	2.37	0.48
1:B:43:LYS:HG3	1:B:43:LYS:O	2.12	0.48
2:D:54:TYR:CD1	2:D:54:TYR:C	2.87	0.47
1:A:31:LEU:HD23	1:A:32:ASN:O	2.13	0.47
1:A:9:LEU:HA	1:A:74:TYR:CE2	2.49	0.47
2:C:68:HIS:C	2:C:70:LYS:H	2.18	0.47
1:A:36:GLN:HE21	1:A:168:ASP:HB2	1.78	0.47
1:A:154:ASN:HA	1:A:199:TYR:CD1	2.50	0.47
1:B:9:LEU:C	1:B:11:ASN:N	2.64	0.47
1:A:8:LYS:CD	1:A:11:ASN:HB3	2.44	0.47
2:D:30:ASP:OD1	2:D:30:ASP:C	2.53	0.47
1:B:88:TRP:O	1:B:88:TRP:HE3	1.96	0.47
1:B:87:VAL:CG2	1:B:89:ARG:HE	2.28	0.47
2:C:62:THR:HB	2:C:65:CYS:HB3	1.96	0.47
1:B:88:TRP:O	1:B:89:ARG:CD	2.63	0.46
1:A:12:ASP:HB2	1:A:14:PHE:CD2	2.49	0.46
1:B:169:LEU:HD12	1:B:170:SER:H	1.80	0.46
1:A:55:TYR:O	1:A:56:LEU:HD23	2.15	0.46
1:A:160:ILE:CD1	1:A:202:VAL:HG13	2.46	0.46
1:A:193:GLY:N	2:C:38:LYS:O	2.29	0.46
1:A:194:CYS:HB3	2:C:37:GLY:H	1.80	0.46
1:B:25:GLU:HB2	1:B:29:LYS:HZ3	1.81	0.46
1:A:177:GLU:O	1:A:210:ARG:NE	2.48	0.46
1:A:15:GLU:OE1	1:A:15:GLU:N	2.49	0.46
1:B:33:VAL:HG22	1:B:62:TRP:HB3	1.98	0.46
1:A:192:TYR:HD2	1:A:199:TYR:HD2	1.63	0.46
1:B:177:GLU:CD	1:B:211:ARG:NH2	2.69	0.46
2:C:52:LYS:HB3	2:C:53:PRO:CD	2.45	0.46
2:D:38:LYS:HE3	2:D:54:TYR:CZ	2.49	0.46
1:B:9:LEU:CA	1:B:11:ASN:H	2.29	0.46
1:A:174:GLU:HB2	1:B:176:VAL:HG23	1.98	0.46
1:A:69:TRP:CZ3	1:A:114:TYR:HA	2.51	0.46
1:A:113:ARG:HB3	1:A:115:ASP:OD1	2.16	0.45
1:B:67:LEU:HB3	1:B:112:LEU:HD21	1.97	0.45
1:A:209:LYS:CG	1:A:210:ARG:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD13	1:B:41:GLN:CG	2.46	0.45
1:B:21:LEU:HD12	1:B:22:ARG:N	2.32	0.45
2:C:51:LYS:HG3	2:C:52:LYS:CB	2.47	0.45
1:A:41:GLN:HB2	1:B:173:ILE:CD1	2.43	0.45
1:A:177:GLU:C	1:A:210:ARG:HE	2.20	0.45
1:A:11:ASN:OD1	1:A:12:ASP:HA	2.16	0.45
2:C:62:THR:HG22	2:C:63:ASP:O	2.16	0.45
2:D:1:ILE:HD11	2:D:62:THR:C	2.37	0.45
1:B:132:VAL:HG22	1:B:133:ASP:N	2.32	0.45
1:B:90:PRO:O	1:B:92:ILE:N	2.48	0.45
1:A:18:SER:O	1:A:20:ALA:N	2.49	0.45
2:D:51:LYS:HE3	2:D:51:LYS:HB3	1.37	0.45
1:B:8:LYS:O	1:B:11:ASN:HB3	2.16	0.45
1:A:39:LEU:HA	1:A:56:LEU:HD22	1.97	0.45
1:B:208:LEU:CA	1:B:209:LYS:HZ3	2.30	0.45
1:A:209:LYS:CD	1:A:210:ARG:N	2.71	0.45
1:B:21:LEU:HD12	1:B:22:ARG:H	1.82	0.44
1:B:8:LYS:HG3	1:B:11:ASN:N	2.32	0.44
1:B:133:ASP:C	1:B:133:ASP:OD1	2.53	0.44
2:C:68:HIS:O	2:C:70:LYS:HG2	2.17	0.44
2:D:72:ARG:HD3	2:D:72:ARG:HH11	1.56	0.44
1:A:12:ASP:CG	1:A:14:PHE:HB2	2.37	0.44
1:B:177:GLU:HG2	1:B:178:TRP:C	2.36	0.44
1:A:171:ASP:OD1	1:B:43:LYS:NZ	2.51	0.44
1:B:19:ASN:O	1:B:88:TRP:HA	2.17	0.44
2:D:51:LYS:NZ	2:D:57:VAL:N	2.56	0.44
2:C:51:LYS:CD	2:C:55:GLU:HG3	2.47	0.44
1:A:194:CYS:SG	2:C:36:ARG:HB2	2.58	0.44
1:A:50:GLN:HE21	1:A:142:GLN:NE2	2.16	0.44
1:B:154:ASN:HB3	1:B:199:TYR:CE1	2.53	0.43
2:D:6:THR:HA	2:D:11:ILE:CD1	2.48	0.43
1:B:110:VAL:HG12	1:B:120:TRP:CD1	2.53	0.43
1:A:210:ARG:CA	1:A:210:ARG:HH11	2.17	0.43
2:D:27:MET:HA	2:D:39:VAL:O	2.17	0.43
1:B:134:VAL:HG13	1:B:139:PHE:HB3	2.00	0.43
1:B:26:ASP:OD1	1:B:29:LYS:HD2	2.19	0.43
1:B:140:ASP:H	1:B:141:ASN:HD22	1.67	0.43
1:A:96:ASN:HB2	1:A:147:THR:H	1.84	0.43
1:A:8:LYS:HD2	1:A:11:ASN:CB	2.46	0.43
1:A:92:ILE:HA	1:A:150:SER:HA	2.01	0.43
1:B:22:ARG:HD2	1:B:153:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:OD1	1:A:11:ASN:N	2.52	0.43
2:C:51:LYS:CG	2:C:55:GLU:HG3	2.48	0.42
2:C:51:LYS:HG3	2:C:52:LYS:HB2	1.99	0.42
2:D:8:THR:CG2	2:D:10:PRO:O	2.66	0.42
2:C:51:LYS:HZ2	2:C:57:VAL:HG11	1.81	0.42
1:A:81:ARG:HA	1:A:110:VAL:O	2.19	0.42
1:B:88:TRP:O	1:B:89:ARG:NE	2.53	0.42
1:B:141:ASN:HA	1:B:209:LYS:CD	2.49	0.42
1:B:62:TRP:NE1	1:B:89:ARG:NH1	2.65	0.42
1:B:89:ARG:HB3	1:B:90:PRO:HD2	2.02	0.42
2:D:51:LYS:CE	2:D:55:GLU:CB	2.90	0.42
1:B:106:VAL:HG13	1:B:123:PRO:HG2	2.00	0.42
1:B:87:VAL:HG23	1:B:89:ARG:CG	2.50	0.42
1:A:189:VAL:HG11	2:C:9:SER:HB2	2.02	0.42
1:B:87:VAL:HB	1:B:89:ARG:HH21	1.83	0.42
1:B:14:PHE:HA	1:B:17:TYR:HB3	2.02	0.42
1:B:12:ASP:OD1	1:B:15:GLU:HB2	2.20	0.42
2:D:29:CYS:SG	2:D:38:LYS:HE2	2.59	0.42
1:A:12:ASP:CB	1:A:14:PHE:HD2	2.31	0.42
1:A:33:VAL:HG21	1:A:90:PRO:HG3	2.00	0.42
1:B:183:MET:HA	1:B:205:THR:O	2.19	0.42
1:B:32:ASN:HB3	1:B:161:PHE:CE2	2.55	0.42
1:B:199:TYR:HE2	2:D:36:ARG:NH1	2.17	0.42
1:A:35:LEU:O	1:A:162:ASN:HA	2.19	0.42
1:B:32:ASN:HB3	1:B:161:PHE:HE2	1.85	0.42
2:D:38:LYS:CE	2:D:54:TYR:CE1	3.01	0.41
2:D:28:TRP:C	2:D:38:LYS:HE2	2.41	0.41
1:A:194:CYS:SG	1:A:195:CYS:N	2.93	0.41
1:A:192:TYR:CD2	1:A:199:TYR:HD2	2.36	0.41
1:A:82:ILE:O	1:A:110:VAL:HG22	2.20	0.41
1:B:88:TRP:CE3	1:B:89:ARG:HA	2.55	0.41
1:B:192:TYR:HB3	1:B:194:CYS:SG	2.61	0.41
1:B:106:VAL:HG22	1:B:106:VAL:O	2.21	0.41
3:B:1214:NAG:H2	3:B:1214:NAG:H61	2.00	0.41
2:C:22:LEU:HD13	2:C:59:CYS:SG	2.61	0.41
2:C:29:CYS:SG	2:C:54:TYR:OH	2.58	0.41
1:A:160:ILE:HD12	1:A:202:VAL:HG13	2.02	0.41
1:B:48:ARG:HH11	1:B:48:ARG:HG2	1.84	0.41
1:A:209:LYS:CG	1:A:210:ARG:H	2.33	0.41
1:A:78:ASP:C	1:A:78:ASP:OD1	2.59	0.41
1:B:140:ASP:O	1:B:140:ASP:CG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:HA	1:B:209:LYS:HD3	1.12	0.41
1:B:131:VAL:O	1:B:142:GLN:HA	2.21	0.41
2:D:27:MET:O	2:D:38:LYS:NZ	2.54	0.41
2:D:54:TYR:CD1	2:D:54:TYR:O	2.74	0.41
1:B:19:ASN:HB2	1:B:88:TRP:HA	2.03	0.41
2:D:70:LYS:HG3	2:D:71:GLN:N	2.27	0.41
2:C:1:ILE:HG23	2:C:16:CYS:SG	2.61	0.41
1:A:10:PHE:O	1:A:10:PHE:CG	2.75	0.40
1:B:208:LEU:O	1:B:209:LYS:CG	2.64	0.40
2:C:68:HIS:C	2:C:70:LYS:N	2.74	0.40
2:C:27:MET:HB3	2:C:38:LYS:HG3	2.02	0.40
1:B:177:GLU:HB3	1:B:179:GLU:OE1	2.21	0.40
2:D:62:THR:HG22	2:D:65:CYS:HB3	2.02	0.40
1:B:162:ASN:OD1	1:B:162:ASN:N	2.53	0.40

There are no symmetry-related clashes.

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	199/218 (91%)	166 (83%)	19 (10%)	14 (7%)	1	2
1	B	199/218 (91%)	168 (84%)	19 (10%)	12 (6%)	2	3
2	C	71/74 (96%)	56 (79%)	9 (13%)	6 (8%)	1	1
2	D	71/74 (96%)	58 (82%)	5 (7%)	8 (11%)	0	0
All	All	540/584 (92%)	448 (83%)	52 (10%)	40 (7%)	1	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	106	VAL
1	A	138	PRO
1	A	170	SER
1	A	174	GLU
1	A	195	CYS
1	B	11	ASN
1	B	97	LYS
1	B	106	VAL
1	B	170	SER
1	B	177	GLU
1	B	196	SER
1	B	209	LYS
1	B	210	ARG
2	C	30	ASP
2	C	52	LYS
2	D	52	LYS
2	D	72	ARG
1	A	12	ASP
1	A	139	PHE
2	C	51	LYS
2	D	31	VAL
2	D	37	GLY
2	D	50	SER
1	A	17	TYR
1	B	192	TYR
2	C	38	LYS
2	D	70	LYS
1	A	11	ASN
1	A	192	TYR
1	B	197	GLU
2	D	7	ALA
1	B	46	ASP
2	C	70	LYS
1	A	46	ASP
1	A	91	ASP
1	B	7	GLN
2	C	69	PRO
2	D	69	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	186/200 (93%)	177 (95%)	9 (5%)	31 62
1	B	186/200 (93%)	171 (92%)	15 (8%)	15 33
2	C	66/66 (100%)	58 (88%)	8 (12%)	6 14
2	D	66/66 (100%)	61 (92%)	5 (8%)	16 37
All	All	504/532 (95%)	467 (93%)	37 (7%)	17 39

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	48	ARG
1	A	79	SER
1	A	89	ARG
1	A	134	VAL
1	A	179	GLU
1	A	191	SER
1	A	197	GLU
1	A	210	ARG
1	B	8	LYS
1	B	24	VAL
1	B	29	LYS
1	B	36	GLN
1	B	43	LYS
1	B	89	ARG
1	B	93	VAL
1	B	106	VAL
1	B	127	LYS
1	B	135	THR
1	B	157	GLN
1	B	158	VAL
1	B	169	LEU
1	B	209	LYS
1	B	212	SER

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Mol	Chain	Res	Type
2	C	1	ILE
2	C	6	THR
2	C	33	CYS
2	C	39	VAL
2	C	51	LYS
2	C	58	THR
2	C	59	CYS
2	C	72	ARG
2	D	8	THR
2	D	34	SER
2	D	51	LYS
2	D	54	TYR
2	D	62	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	50	GLN
1	B	7	GLN
1	B	36	GLN
1	B	50	GLN
1	B	141	ASN
2	D	21	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

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	NAG	A	1214	1	14,14,15	0.50	0	15,19,21	1.22	1 (6%)
3	NAG	A	1215	1	14,14,15	0.91	1 (7%)	15,19,21	0.76	0
3	NAG	B	1214	1	14,14,15	0.82	1 (7%)	15,19,21	1.22	1 (6%)
3	NAG	B	1215	1	14,14,15	0.52	0	15,19,21	0.71	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
3	NAG	A	1214	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1214	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1215	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1215	NAG	O5-C1	-3.14	1.38	1.43
3	B	1214	NAG	O5-C1	2.87	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1214	NAG	C1-O5-C5	3.30	116.43	112.25
3	A	1214	NAG	C1-O5-C5	4.30	117.70	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1214	NAG	1	0
3	B	1214	NAG	2	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	203/218 (93%)	0.89	20 (9%) 9 7	47, 97, 173, 220	0
1	B	203/218 (93%)	0.85	21 (10%) 9 6	60, 107, 171, 232	0
2	C	73/74 (98%)	0.66	6 (8%) 14 11	68, 97, 174, 192	0
2	D	73/74 (98%)	0.56	4 (5%) 29 27	76, 103, 170, 198	0
All	All	552/584 (94%)	0.80	51 (9%) 11 9	47, 101, 177, 232	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	73	PRO	8.0
1	A	13	LEU	5.9
1	B	12	ASP	5.8
1	A	139	PHE	5.3
1	B	178	TRP	5.3
1	A	138	PRO	5.1
1	B	13	LEU	5.0
1	A	12	ASP	4.3
2	D	72	ARG	4.2
1	A	25	GLU	3.8
1	A	196	SER	3.8
1	A	134	VAL	3.6
1	B	141	ASN	3.5
2	C	72	ARG	3.5
1	A	74	TYR	3.3
1	A	137	PHE	3.3
1	A	133	ASP	3.1
1	B	134	VAL	3.0
1	B	137	PHE	3.0
1	B	41	GLN	2.8
1	B	180	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	105	PRO	2.7
1	A	178	TRP	2.7
1	B	146	LEU	2.7
1	B	176	VAL	2.7
1	B	105	PRO	2.6
1	A	14	PHE	2.6
2	D	73	PRO	2.6
1	B	202	VAL	2.6
1	B	207	LEU	2.4
1	B	58	ILE	2.4
1	A	140	ASP	2.4
1	A	72	ASP	2.4
1	A	158	VAL	2.4
1	B	181	HIS	2.3
1	A	66	TYR	2.3
1	A	207	LEU	2.2
2	C	14	VAL	2.2
2	D	14	VAL	2.2
1	A	42	ILE	2.2
1	B	155	GLY	2.2
1	B	92	ILE	2.1
1	B	33	VAL	2.1
2	C	54	TYR	2.1
2	D	1	ILE	2.1
1	B	177	GLU	2.1
2	C	31	VAL	2.1
2	C	28	TRP	2.0
1	A	146	LEU	2.0
1	B	28	ASP	2.0
1	B	42	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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	1215	14/15	0.89	0.18	-0.79	104,114,129,149	0
3	NAG	B	1214	14/15	0.85	0.17	-1.11	106,123,150,151	0
3	NAG	B	1215	14/15	0.90	0.17	-1.29	99,114,124,133	0
3	NAG	A	1214	14/15	0.91	0.14	-1.47	75,105,115,123	0

6.5 Other polymers

There are no such residues in this entry.