Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:51 PM GMT

PDB ID	:	4DOH
Title	:	IL20/IL201/IL20R2 Ternary Complex
Authors	:	Logsdon, N.J.; Walter, M.R.
Deposited on	:	2012-02-09
Resolution	:	2.80 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:

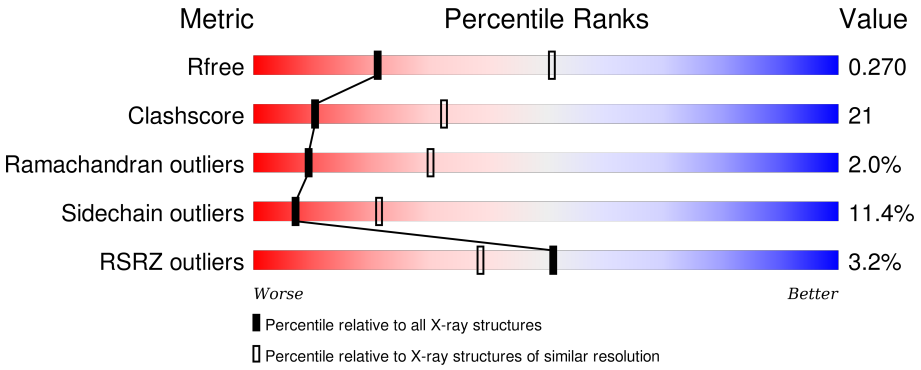
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	153	% 71% 23% 7%
1	C	153	75% 22% .
2	B	206	% 68% 19% 6% 6%
2	D	206	5% 57% 30% 7% 6%
3	E	221	5% 50% 35% 7% 8%

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Mol	Chain	Length	Quality of chain
3	R	221	

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	R	302	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8949 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 Interleukin-20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1231	772	224	226	9			
1	C	153	Total	C	N	O	S	0	0	0
			1231	772	224	226	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	EXPRESSION TAG	UNP Q9NYY1
C	24	ALA	-	EXPRESSION TAG	UNP Q9NYY1

- Molecule 2 is a protein called Interleukin-20 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1525	977	251	288	9			
2	D	193	Total	C	N	O	S	0	0	0
			1525	977	251	288	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ALA	-	EXPRESSION TAG	UNP Q6UXL0
B	40	GLN	ASN	ENGINEERED MUTATION	UNP Q6UXL0
B	134	GLN	ASN	ENGINEERED MUTATION	UNP Q6UXL0
B	232	GLU	-	EXPRESSION TAG	UNP Q6UXL0
B	233	GLY	-	EXPRESSION TAG	UNP Q6UXL0
B	234	ARG	-	EXPRESSION TAG	UNP Q6UXL0
D	29	ALA	-	EXPRESSION TAG	UNP Q6UXL0
D	40	GLN	ASN	ENGINEERED MUTATION	UNP Q6UXL0
D	134	GLN	ASN	ENGINEERED MUTATION	UNP Q6UXL0
D	232	GLU	-	EXPRESSION TAG	UNP Q6UXL0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	233	GLY	-	EXPRESSION TAG	UNP Q6UXL0
D	234	ARG	-	EXPRESSION TAG	UNP Q6UXL0

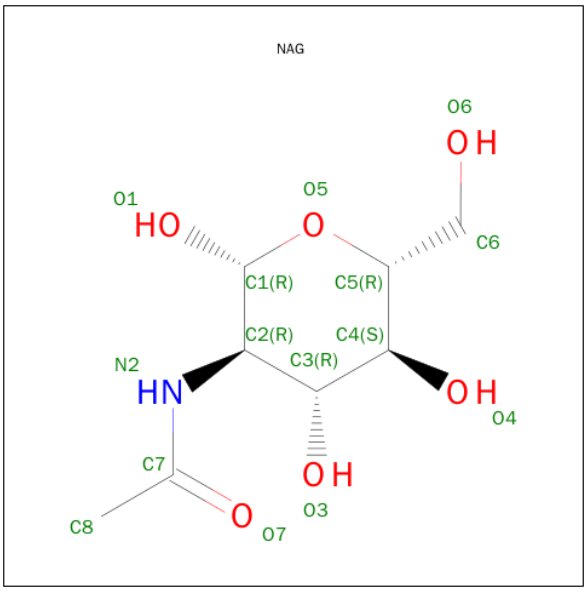
- Molecule 3 is a protein called Interleukin-20 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	204	Total	C	N	O	S	0	0	0
			1655	1055	284	308	8			
3	E	204	Total	C	N	O	S	0	0	0
			1655	1055	284	308	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	111	ARG	LYS	ENGINEERED MUTATION	UNP Q9UHF4
R	113	ARG	LYS	ENGINEERED MUTATION	UNP Q9UHF4
R	246	ILE	-	EXPRESSION TAG	UNP Q9UHF4
R	247	GLU	-	EXPRESSION TAG	UNP Q9UHF4
R	248	GLY	-	EXPRESSION TAG	UNP Q9UHF4
R	249	ARG	-	EXPRESSION TAG	UNP Q9UHF4
E	111	ARG	LYS	ENGINEERED MUTATION	UNP Q9UHF4
E	113	ARG	LYS	ENGINEERED MUTATION	UNP Q9UHF4
E	246	ILE	-	EXPRESSION TAG	UNP Q9UHF4
E	247	GLU	-	EXPRESSION TAG	UNP Q9UHF4
E	248	GLY	-	EXPRESSION TAG	UNP Q9UHF4
E	249	ARG	-	EXPRESSION TAG	UNP Q9UHF4

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	R	1	Total C N O 14 8 1 5	0	0
4	R	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

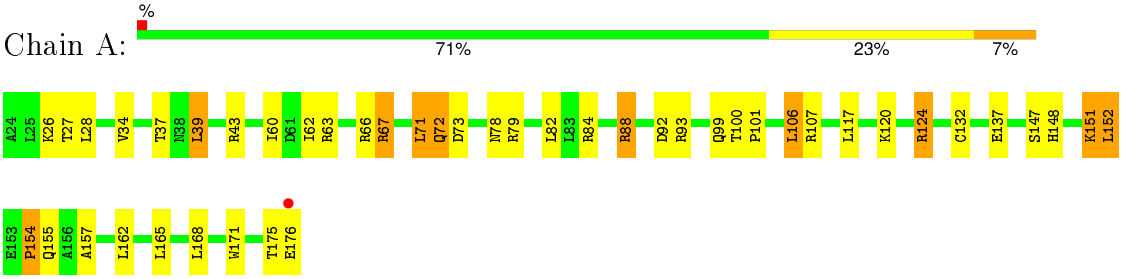
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	14	Total O 14 14	0	0
5	R	6	Total O 6 6	0	0
5	C	16	Total O 16 16	0	0
5	D	6	Total O 6 6	0	0
5	E	8	Total O 8 8	0	0

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.

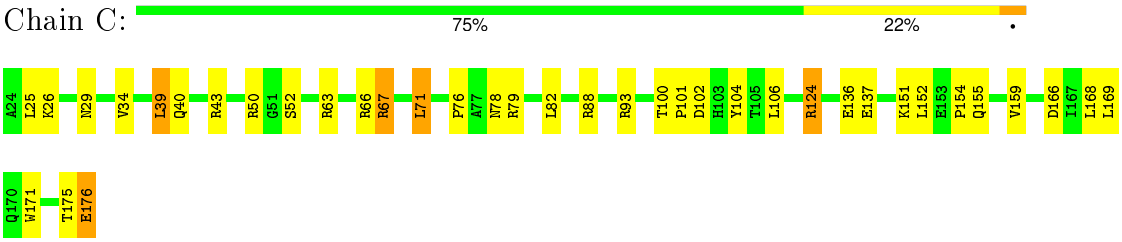
- Molecule 1: Interleukin-20

Chain A:



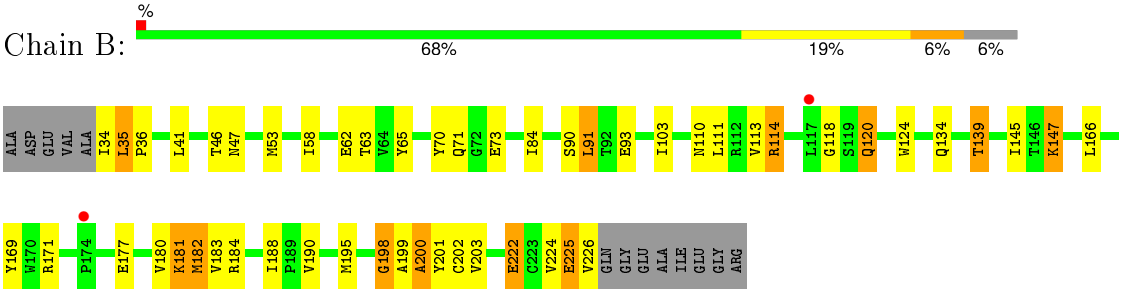
- Molecule 1: Interleukin-20

Chain C:



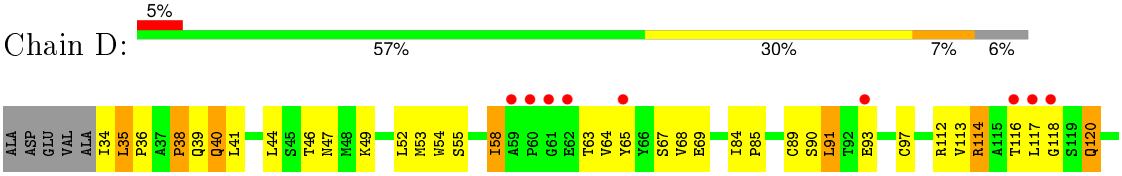
- Molecule 2: Interleukin-20 receptor subunit beta

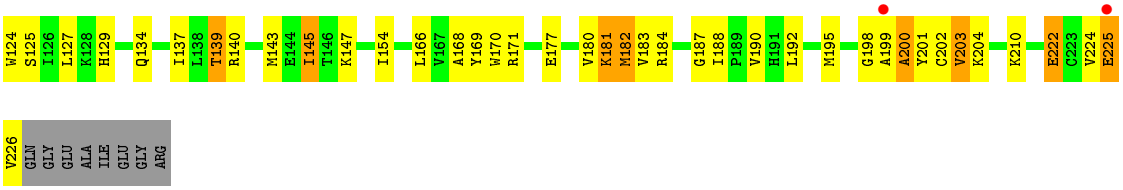
Chain B:



- Molecule 2: Interleukin-20 receptor subunit beta

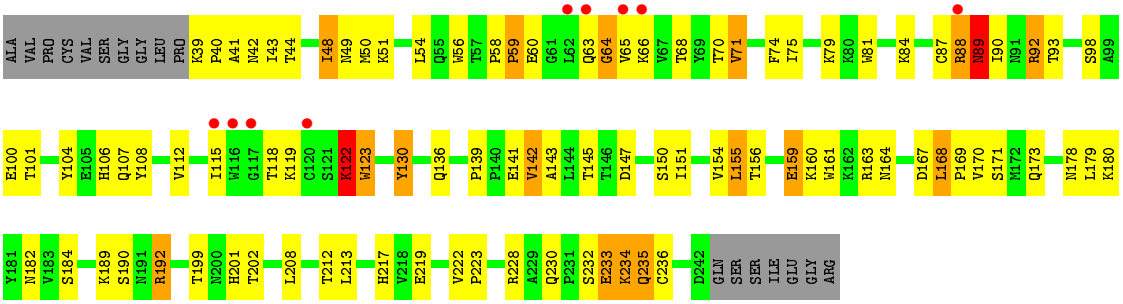
Chain D:





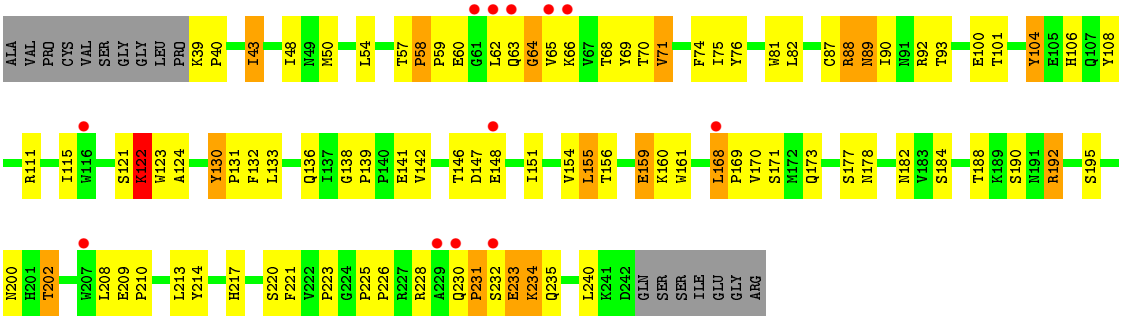
• Molecule 3: Interleukin-20 receptor subunit alpha

Chain R:



• Molecule 3: Interleukin-20 receptor subunit alpha

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.11Å 111.76Å 136.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.13 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 96.5 (49.13-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.278 0.211 , 0.270	Depositor DCC
R_{free} test set	1952 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 38635 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8949	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: 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	0.50	0/1249	0.66	0/1678
1	C	0.48	0/1249	0.63	0/1678
2	B	0.45	0/1568	0.63	0/2140
2	D	0.46	0/1568	0.65	0/2140
3	E	0.48	0/1701	0.64	0/2322
3	R	0.47	0/1701	0.64	0/2322
All	All	0.47	0/9036	0.64	0/12280

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	198	GLY	Peptide
2	D	187	GLY	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	1231	0	1253	39	0
1	C	1231	0	1253	25	0
2	B	1525	0	1479	58	0
2	D	1525	0	1479	72	0
3	E	1655	0	1618	100	0
3	R	1655	0	1618	90	0
4	B	14	0	13	2	0
4	D	14	0	13	1	0
4	E	14	0	13	4	0
4	R	28	0	26	9	0
5	A	7	0	0	3	0
5	B	14	0	0	0	0
5	C	16	0	0	0	0
5	D	6	0	0	0	0
5	E	8	0	0	1	0
5	R	6	0	0	0	0
All	All	8949	0	8765	377	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 21.

All (377) 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:C:124:ARG:HH11	1:C:124:ARG:HG3	1.12	1.14
3:E:182:ASN:ND2	4:E:301:NAG:C1	2.14	1.10
3:E:70:THR:HG22	3:E:89:ASN:H	1.18	1.08
2:B:171:ARG:HH22	2:B:198:GLY:HA3	1.19	1.07
1:A:66:ARG:O	1:A:67:ARG:HB3	1.57	1.02
3:R:192:ARG:HH11	3:R:192:ARG:HG2	1.26	1.00
3:E:138:GLY:HA2	3:E:230:GLN:HG2	1.42	0.99
3:R:42:ASN:HD21	4:R:301:NAG:C1	1.77	0.97
3:E:192:ARG:HG2	3:E:192:ARG:HH11	1.31	0.95
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.33	0.91
2:D:147:LYS:HD3	2:D:226:VAL:HG22	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ARG:NH2	2:B:198:GLY:HA3	1.88	0.86
2:D:225:GLU:CD	2:D:226:VAL:H	1.77	0.86
2:B:225:GLU:CD	2:B:226:VAL:H	1.79	0.85
3:E:148:GLU:HB3	3:E:240:LEU:HB2	1.58	0.85
3:E:104:TYR:HB3	3:E:132:PHE:HB2	1.58	0.83
3:R:63:GLN:HE21	3:R:64:GLY:H	1.25	0.83
3:R:219:GLU:HG2	3:R:232:SER:HB3	1.59	0.83
3:E:182:ASN:HD22	4:E:301:NAG:C1	1.87	0.82
1:A:124:ARG:HH11	1:A:124:ARG:CG	1.91	0.81
3:R:70:THR:HG22	3:R:88:ARG:HA	1.62	0.80
3:E:147:ASP:CG	3:E:148:GLU:H	1.84	0.80
3:E:68:THR:HG23	3:E:90:ILE:O	1.82	0.80
3:E:192:ARG:CG	3:E:192:ARG:HH11	1.95	0.80
3:E:192:ARG:HG2	3:E:192:ARG:NH1	1.92	0.79
3:E:58:PRO:HD3	3:E:93:THR:HG21	1.62	0.79
2:D:171:ARG:HH22	2:D:198:GLY:HA3	1.46	0.79
1:C:124:ARG:NH1	1:C:124:ARG:HG3	1.84	0.79
3:E:178:ASN:HD22	3:E:223:PRO:HG2	1.47	0.79
2:D:46:THR:HG22	2:D:137:ILE:HB	1.65	0.78
2:D:64:VAL:HG22	2:D:117:LEU:HG	1.66	0.78
3:E:70:THR:CG2	3:E:89:ASN:H	1.97	0.78
3:E:234:LYS:H	3:E:234:LYS:HD2	1.49	0.77
3:R:182:ASN:ND2	4:R:302:NAG:C1	2.49	0.76
1:C:124:ARG:HH11	1:C:124:ARG:CG	1.94	0.76
1:A:124:ARG:NH1	1:A:124:ARG:HG3	1.95	0.76
3:R:42:ASN:ND2	4:R:301:NAG:C1	2.48	0.75
3:E:39:LYS:HA	3:E:122:LYS:NZ	2.01	0.75
3:R:233:GLU:HA	3:R:233:GLU:OE1	1.85	0.75
3:E:43:ILE:H	3:E:43:ILE:HD12	1.52	0.74
1:C:78:ASN:ND2	1:C:137:GLU:HB3	2.02	0.74
2:D:171:ARG:HG3	2:D:199:ALA:HB3	1.70	0.73
4:B:301:NAG:H2	4:R:302:NAG:O4	1.89	0.73
3:E:182:ASN:HD21	4:E:301:NAG:C1	2.01	0.72
3:R:143:ALA:HB3	3:R:154:VAL:HG23	1.69	0.72
3:R:233:GLU:CD	3:R:234:LYS:H	1.93	0.72
2:D:145:ILE:H	2:D:145:ILE:HD12	1.53	0.72
2:D:40:GLN:O	2:D:54:TRP:HA	1.89	0.72
3:E:70:THR:HG22	3:E:89:ASN:N	2.02	0.71
3:E:178:ASN:ND2	3:E:223:PRO:HG2	2.04	0.71
3:E:159:GLU:OE2	3:E:169:PRO:HB3	1.88	0.71
2:D:199:ALA:O	2:D:200:ALA:CB	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:192:ARG:HG2	3:R:192:ARG:NH1	1.94	0.70
2:B:145:ILE:HG12	2:B:203:VAL:HG21	1.73	0.70
3:E:68:THR:HB	3:E:115:ILE:HD11	1.71	0.70
3:R:70:THR:CG2	3:R:89:ASN:H	2.04	0.70
3:R:39:LYS:N	3:R:40:PRO:HD3	2.06	0.70
3:R:182:ASN:HD21	4:R:302:NAG:C1	2.05	0.70
3:E:154:VAL:HG12	3:E:202:THR:HB	1.74	0.69
3:R:63:GLN:NE2	3:R:64:GLY:H	1.90	0.69
2:B:41:LEU:HD21	2:B:113:VAL:HG12	1.74	0.69
2:D:199:ALA:O	2:D:200:ALA:HB3	1.92	0.69
2:B:195:MET:HE1	2:B:224:VAL:HG23	1.75	0.68
2:B:188:ILE:CD1	4:R:302:NAG:H3	2.24	0.68
3:E:39:LYS:N	3:E:40:PRO:HD3	2.09	0.68
3:E:63:GLN:HG2	3:E:64:GLY:H	1.59	0.68
1:A:78:ASN:ND2	1:A:137:GLU:HB3	2.07	0.68
3:R:74:PHE:HB2	3:R:81:TRP:CE3	2.29	0.67
3:R:58:PRO:HD3	3:R:93:THR:HG21	1.76	0.67
3:E:233:GLU:HA	3:E:233:GLU:OE1	1.94	0.67
3:E:139:PRO:HG3	3:E:231:PRO:O	1.93	0.67
2:D:188:ILE:HD13	4:E:301:NAG:H3	1.77	0.67
1:C:66:ARG:O	1:C:67:ARG:HB3	1.95	0.67
2:B:200:ALA:HA	2:B:225:GLU:HG2	1.77	0.67
3:R:190:SER:HB2	3:R:192:ARG:HG3	1.77	0.66
3:R:192:ARG:HH11	3:R:192:ARG:CG	2.05	0.66
2:B:188:ILE:HD11	4:R:302:NAG:H3	1.78	0.66
2:D:84:ILE:HG23	2:D:85:PRO:HD2	1.77	0.65
2:D:34:ILE:HD12	2:D:35:LEU:N	2.12	0.65
1:A:28:LEU:HD12	1:A:37:THR:HG21	1.79	0.65
2:D:34:ILE:HG13	2:D:120:GLN:HE21	1.61	0.65
3:R:71:VAL:HG13	3:R:87:CYS:HB3	1.79	0.65
1:C:66:ARG:O	1:C:67:ARG:CB	2.45	0.64
3:R:233:GLU:OE2	3:R:234:LYS:HD2	1.96	0.64
2:D:195:MET:HE1	2:D:224:VAL:HG23	1.79	0.64
1:A:100:THR:CG2	1:A:106:LEU:HD13	2.28	0.64
3:R:74:PHE:HB2	3:R:81:TRP:CZ3	2.33	0.64
2:D:143:MET:HE1	2:D:203:VAL:HG23	1.79	0.63
2:D:145:ILE:N	2:D:145:ILE:HD12	2.12	0.63
1:A:78:ASN:HD22	1:A:137:GLU:HB3	1.62	0.63
4:B:301:NAG:C2	4:R:302:NAG:O4	2.46	0.63
3:E:43:ILE:HG22	3:E:54:LEU:HD11	1.80	0.63
3:R:43:ILE:HD12	3:R:43:ILE:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:49:ASN:O	3:R:50:MET:HB2	2.00	0.62
3:R:155:LEU:HD12	3:R:201:HIS:O	2.01	0.61
3:R:70:THR:HG22	3:R:89:ASN:H	1.64	0.61
3:E:101:THR:HG22	3:E:108:TYR:CG	2.36	0.61
3:E:147:ASP:CG	3:E:148:GLU:N	2.48	0.61
2:D:41:LEU:HA	2:D:53:MET:O	2.01	0.61
3:E:39:LYS:HA	3:E:122:LYS:HZ2	1.65	0.60
3:R:180:LYS:HG2	3:R:199:THR:HG22	1.83	0.60
3:R:168:LEU:HD12	3:R:168:LEU:H	1.67	0.60
1:C:76:PRO:HA	1:C:79:ARG:HG3	1.81	0.60
1:A:28:LEU:HD12	1:A:37:THR:CG2	2.32	0.59
3:R:159:GLU:OE2	3:R:169:PRO:HB3	2.02	0.59
2:B:199:ALA:O	2:B:200:ALA:HB3	2.01	0.59
2:B:169:TYR:HB3	2:B:203:VAL:HG12	1.84	0.59
2:B:200:ALA:CA	2:B:225:GLU:HG2	2.33	0.59
3:E:111:ARG:HA	3:E:124:ALA:O	2.02	0.58
2:B:145:ILE:HD12	2:B:145:ILE:N	2.18	0.58
3:E:62:LEU:HB2	3:E:63:GLN:OE1	2.03	0.58
3:R:173:GLN:HG3	3:R:179:LEU:HB3	1.85	0.58
1:A:43:ARG:HD2	5:A:202:HOH:O	2.02	0.58
3:E:63:GLN:H	3:E:63:GLN:NE2	2.02	0.58
1:A:99:GLN:HG2	1:A:155:GLN:OE1	2.03	0.58
2:D:34:ILE:HG13	2:D:120:GLN:NE2	2.17	0.58
3:E:136:GLN:HE21	3:E:228:ARG:HD3	1.69	0.57
3:R:178:ASN:HD22	3:R:223:PRO:HG2	1.68	0.57
3:R:136:GLN:HE21	3:R:228:ARG:HD3	1.68	0.57
2:D:39:GLN:OE1	2:D:39:GLN:HA	2.05	0.57
2:B:34:ILE:HD12	2:B:35:LEU:N	2.19	0.57
1:C:26:LYS:NZ	1:C:176:GLU:O	2.27	0.56
2:D:35:LEU:HD23	2:D:36:PRO:HD2	1.87	0.56
2:D:195:MET:HB3	2:D:201:TYR:CE2	2.41	0.56
2:D:90:SER:O	2:D:91:LEU:HB2	2.06	0.56
4:D:301:NAG:C1	4:D:301:NAG:O4	2.53	0.56
3:E:148:GLU:CB	3:E:240:LEU:HB2	2.31	0.56
2:D:166:LEU:CD2	2:D:182:MET:HG2	2.36	0.56
2:B:47:ASN:HD21	2:B:139:THR:HB	1.70	0.56
2:D:171:ARG:CG	2:D:199:ALA:HB3	2.36	0.55
2:D:35:LEU:HD11	2:D:117:LEU:HB2	1.88	0.55
2:B:166:LEU:HD23	2:B:182:MET:HG2	1.88	0.55
2:D:181:LYS:HG3	2:D:182:MET:N	2.21	0.55
2:B:103:ILE:N	2:B:103:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ILE:HG12	2:B:203:VAL:CG2	2.37	0.55
3:E:63:GLN:HG2	3:E:64:GLY:N	2.21	0.54
3:R:68:THR:HG22	3:R:90:ILE:N	2.21	0.54
2:D:112:ARG:HG3	2:D:124:TRP:CE3	2.42	0.54
3:E:168:LEU:HD12	3:E:168:LEU:H	1.72	0.54
3:E:74:PHE:CD2	3:E:75:ILE:N	2.75	0.54
3:E:190:SER:OG	3:E:192:ARG:HG3	2.08	0.54
2:D:200:ALA:CA	2:D:225:GLU:HG2	2.37	0.54
3:R:222:VAL:HG23	3:R:222:VAL:O	2.07	0.54
2:B:84:ILE:N	2:B:84:ILE:HD12	2.22	0.54
2:D:225:GLU:CD	2:D:226:VAL:N	2.55	0.54
3:E:141:GLU:O	3:E:155:LEU:HA	2.08	0.54
3:E:136:GLN:HG2	3:E:228:ARG:HB2	1.89	0.54
3:R:63:GLN:HG2	3:R:64:GLY:N	2.23	0.53
2:D:69:GLU:OE1	2:D:112:ARG:NH2	2.39	0.53
3:E:68:THR:HG22	3:E:69:TYR:N	2.23	0.53
3:R:168:LEU:HD12	3:R:168:LEU:N	2.23	0.53
3:E:104:TYR:CB	3:E:132:PHE:HB2	2.35	0.53
3:R:164:ASN:O	3:R:167:ASP:HB2	2.09	0.53
1:A:71:LEU:HD13	1:A:175:THR:HG21	1.92	0.52
2:B:35:LEU:CD2	2:B:36:PRO:HD2	2.39	0.52
3:E:68:THR:HG21	3:E:89:ASN:OD1	2.09	0.52
2:B:91:LEU:HD22	2:B:91:LEU:N	2.25	0.52
2:D:65:TYR:CE1	2:D:93:GLU:HG2	2.44	0.52
2:D:195:MET:HE1	2:D:224:VAL:CG2	2.39	0.52
2:D:183:VAL:HG13	2:D:190:VAL:HG21	1.90	0.52
2:D:67:SER:OG	2:D:91:LEU:HD22	2.10	0.51
3:R:160:LYS:HG2	3:R:161:TRP:N	2.23	0.51
3:E:160:LYS:HG2	3:E:161:TRP:N	2.24	0.51
2:B:199:ALA:O	2:B:200:ALA:CB	2.58	0.51
2:D:34:ILE:HD12	2:D:35:LEU:H	1.75	0.51
2:D:169:TYR:HA	2:D:202:CYS:O	2.10	0.51
3:R:151:ILE:HG13	3:R:208:LEU:CD1	2.41	0.51
1:C:155:GLN:O	1:C:159:VAL:HG23	2.11	0.51
3:R:68:THR:HB	3:R:115:ILE:CG1	2.41	0.51
3:R:70:THR:HG23	3:R:89:ASN:H	1.73	0.51
1:A:84:ARG:HH11	1:A:120:LYS:HZ3	1.57	0.51
2:D:34:ILE:HD11	2:D:120:GLN:HG3	1.93	0.51
3:R:168:LEU:CD1	3:R:168:LEU:H	2.22	0.50
2:D:201:TYR:CD2	2:D:201:TYR:N	2.79	0.50
1:A:124:ARG:HH11	1:A:124:ARG:CB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:HD11	2:B:120:GLN:HG3	1.92	0.50
2:D:200:ALA:HA	2:D:225:GLU:HG2	1.92	0.50
2:D:84:ILE:CG2	2:D:85:PRO:HD2	2.42	0.50
2:B:114:ARG:HG2	2:B:124:TRP:CZ3	2.47	0.50
3:R:234:LYS:O	3:R:234:LYS:HD2	2.12	0.50
3:E:68:THR:HB	3:E:115:ILE:CD1	2.40	0.50
2:B:147:LYS:HE2	2:B:225:GLU:O	2.11	0.50
2:B:145:ILE:HD12	2:B:145:ILE:H	1.76	0.50
2:B:195:MET:HB3	2:B:201:TYR:CE2	2.48	0.49
3:R:48:ILE:O	3:R:48:ILE:HG13	2.13	0.49
1:A:154:PRO:O	1:A:157:ALA:N	2.44	0.49
2:B:65:TYR:CE1	2:B:93:GLU:HG2	2.47	0.49
2:B:70:TYR:HB3	2:B:111:LEU:HD23	1.93	0.49
3:E:115:ILE:C	3:E:115:ILE:HD12	2.33	0.49
5:A:201:HOH:O	3:R:106:HIS:HD2	1.95	0.49
1:A:62:ILE:HD12	1:A:151:LYS:HE3	1.93	0.49
3:E:66:LYS:O	3:E:66:LYS:HG2	2.11	0.49
3:R:118:THR:O	3:R:118:THR:HG22	2.11	0.49
3:R:63:GLN:HG2	3:R:64:GLY:H	1.76	0.49
2:D:38:PRO:HB3	2:D:54:TRP:CD1	2.48	0.49
1:C:67:ARG:NH1	3:E:106:HIS:CE1	2.81	0.49
2:D:91:LEU:HD11	2:D:116:THR:HG21	1.95	0.49
1:A:100:THR:HG23	1:A:106:LEU:HD13	1.95	0.48
3:R:160:LYS:HB3	3:R:170:VAL:HB	1.94	0.48
1:C:40:GLN:NE2	3:E:226:PRO:HD3	2.28	0.48
3:E:69:TYR:CE2	3:E:93:THR:HG22	2.49	0.48
2:B:103:ILE:O	2:B:103:ILE:HG22	2.12	0.48
3:R:63:GLN:CG	3:R:64:GLY:H	2.25	0.48
2:B:188:ILE:HD13	4:R:302:NAG:H3	1.94	0.48
1:A:100:THR:OG1	1:A:101:PRO:HD2	2.13	0.48
3:R:155:LEU:HD12	3:R:155:LEU:H	1.78	0.48
2:D:39:GLN:O	2:D:55:SER:N	2.42	0.48
2:D:171:ARG:NH1	2:D:199:ALA:H	2.12	0.48
2:D:34:ILE:CG1	2:D:120:GLN:HE21	2.26	0.48
1:C:40:GLN:HE22	3:E:226:PRO:HD3	1.77	0.48
3:E:108:TYR:N	3:E:108:TYR:CD2	2.81	0.48
3:E:230:GLN:O	3:E:231:PRO:C	2.52	0.48
3:R:39:LYS:N	3:R:40:PRO:CD	2.75	0.48
2:B:41:LEU:H	2:B:41:LEU:HD12	1.78	0.48
2:B:183:VAL:HG13	2:B:190:VAL:HG21	1.96	0.48
2:D:147:LYS:HE2	2:D:225:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:217:HIS:HB3	3:R:234:LYS:HA	1.96	0.47
2:B:70:TYR:CB	2:B:111:LEU:HD23	2.44	0.47
3:E:63:GLN:CG	3:E:64:GLY:H	2.25	0.47
2:D:41:LEU:HD21	2:D:113:VAL:HG12	1.96	0.47
3:R:178:ASN:ND2	3:R:223:PRO:HG2	2.29	0.47
3:E:90:ILE:HD13	3:E:92:ARG:NH2	2.29	0.47
2:D:64:VAL:HA	2:D:117:LEU:HD23	1.96	0.47
3:R:43:ILE:CG2	3:R:54:LEU:HD11	2.45	0.47
2:B:35:LEU:HD22	2:B:36:PRO:HD2	1.95	0.47
2:B:225:GLU:CD	2:B:226:VAL:N	2.60	0.47
3:E:39:LYS:HA	3:E:122:LYS:HZ3	1.76	0.47
2:D:114:ARG:HG2	2:D:124:TRP:CH2	2.49	0.47
3:R:63:GLN:O	3:R:65:VAL:N	2.48	0.47
3:R:139:PRO:HD3	3:R:230:GLN:HG2	1.97	0.47
3:E:115:ILE:O	3:E:115:ILE:HD12	2.15	0.47
1:A:63:ARG:O	1:A:66:ARG:HG3	2.14	0.47
2:B:145:ILE:HD13	2:B:222:GLU:OE1	2.14	0.47
2:B:195:MET:HE3	2:B:201:TYR:HB2	1.95	0.47
3:E:63:GLN:CD	3:E:63:GLN:N	2.67	0.47
3:E:168:LEU:N	3:E:168:LEU:HD12	2.30	0.47
1:A:34:VAL:HG11	1:C:34:VAL:HG11	1.97	0.47
2:D:192:LEU:HA	2:D:192:LEU:HD23	1.59	0.47
2:D:170:TRP:CE2	2:D:202:CYS:HB2	2.50	0.47
1:C:71:LEU:HD13	1:C:175:THR:HG21	1.97	0.47
2:D:68:VAL:HB	2:D:89:CYS:HB2	1.97	0.47
3:R:40:PRO:HG2	3:R:112:VAL:HG13	1.97	0.47
2:B:195:MET:HE1	2:B:224:VAL:CG2	2.43	0.47
2:B:166:LEU:CD2	2:B:182:MET:HG2	2.45	0.47
3:E:160:LYS:HE3	3:E:161:TRP:O	2.15	0.46
3:E:146:THR:HG22	3:E:151:ILE:HG12	1.97	0.46
3:E:68:THR:HG21	3:E:89:ASN:CG	2.35	0.46
1:A:124:ARG:HH11	1:A:124:ARG:HB2	1.81	0.46
3:E:39:LYS:N	3:E:40:PRO:CD	2.79	0.46
3:E:43:ILE:CG2	3:E:54:LEU:HD11	2.45	0.46
3:E:63:GLN:CD	3:E:63:GLN:H	2.19	0.46
1:A:117:LEU:HD21	2:B:73:GLU:HG2	1.96	0.46
3:E:100:GLU:CD	3:E:100:GLU:H	2.19	0.46
3:R:130:TYR:C	3:R:130:TYR:CD1	2.88	0.46
3:R:63:GLN:CG	3:R:64:GLY:N	2.79	0.46
2:D:166:LEU:HD23	2:D:182:MET:HG2	1.98	0.46
1:A:66:ARG:HD3	1:A:148:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:LEU:CD1	2:D:116:THR:HG21	2.46	0.46
1:C:78:ASN:HD22	1:C:137:GLU:HB3	1.77	0.46
3:R:43:ILE:O	3:R:44:THR:HG23	2.16	0.46
3:R:68:THR:HG21	3:R:89:ASN:OD1	2.16	0.46
3:R:90:ILE:HG21	3:R:92:ARG:HH22	1.80	0.46
1:A:171:TRP:O	1:A:175:THR:HG23	2.16	0.46
2:B:34:ILE:HG13	2:B:120:GLN:NE2	2.31	0.46
3:R:84:LYS:HE2	3:R:100:GLU:CD	2.36	0.46
3:E:104:TYR:CD1	3:E:104:TYR:N	2.85	0.45
3:R:130:TYR:C	3:R:130:TYR:HD1	2.19	0.45
3:R:233:GLU:CD	3:R:234:LYS:N	2.65	0.45
3:E:233:GLU:OE1	3:E:234:LYS:HD2	2.16	0.45
1:A:39:LEU:HA	1:A:39:LEU:HD12	1.71	0.45
2:D:40:GLN:HB2	2:D:55:SER:OG	2.16	0.45
2:B:41:LEU:HA	2:B:53:MET:O	2.16	0.45
3:R:56:TRP:CE2	3:R:93:THR:HA	2.52	0.45
3:R:51:LYS:HA	3:R:98:SER:OG	2.17	0.45
2:D:145:ILE:HD13	2:D:222:GLU:HG2	1.99	0.45
2:D:67:SER:O	2:D:113:VAL:HA	2.16	0.45
3:R:136:GLN:NE2	3:R:228:ARG:HD3	2.32	0.45
2:B:134:GLN:NE2	2:D:134:GLN:NE2	2.65	0.45
1:A:124:ARG:HD2	5:A:205:HOH:O	2.16	0.45
3:R:58:PRO:HA	3:R:59:PRO:HD3	1.82	0.45
2:D:34:ILE:CD1	2:D:120:GLN:HE21	2.30	0.45
2:D:47:ASN:HD21	2:D:139:THR:HB	1.81	0.45
3:R:189:LYS:HB2	3:R:212:THR:HG23	1.98	0.44
3:R:101:THR:HA	3:R:108:TYR:CZ	2.52	0.44
3:R:48:ILE:HD12	3:R:49:ASN:CG	2.37	0.44
3:E:217:HIS:HA	3:E:233:GLU:O	2.17	0.44
1:A:72:GLN:HG3	1:A:73:ASP:N	2.32	0.44
1:A:88:ARG:HD3	1:A:92:ASP:OD2	2.18	0.44
2:B:71:GLN:HE21	2:B:110:ASN:HD22	1.65	0.44
1:A:84:ARG:HH11	1:A:120:LYS:NZ	2.16	0.44
2:D:65:TYR:HE1	2:D:93:GLU:HG2	1.82	0.44
2:B:34:ILE:CD1	2:B:120:GLN:HE21	2.31	0.44
1:C:63:ARG:HG3	3:E:76:TYR:CE2	2.53	0.44
3:E:74:PHE:HB2	3:E:81:TRP:CZ3	2.52	0.44
2:B:71:GLN:HG2	2:B:110:ASN:HB2	1.99	0.44
1:C:171:TRP:O	1:C:175:THR:HG23	2.18	0.43
3:E:88:ARG:HH11	3:E:88:ARG:HB2	1.83	0.43
1:C:100:THR:OG1	1:C:101:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:63:GLN:HE21	3:R:64:GLY:N	2.04	0.43
2:D:143:MET:CE	2:D:203:VAL:HG23	2.46	0.43
2:B:200:ALA:N	2:B:225:GLU:HG2	2.33	0.43
2:B:103:ILE:N	2:B:103:ILE:CD1	2.81	0.43
3:E:225:PRO:HA	3:E:226:PRO:HD2	1.93	0.43
3:E:50:MET:HE1	3:E:131:PRO:HB2	2.00	0.43
3:E:63:GLN:O	3:E:65:VAL:N	2.52	0.43
3:R:171:SER:C	3:R:173:GLN:N	2.72	0.43
3:E:141:GLU:HG2	3:E:156:THR:OG1	2.19	0.43
3:E:71:VAL:HG13	3:E:87:CYS:HB3	2.01	0.43
1:A:100:THR:HG22	1:A:106:LEU:HD13	2.00	0.43
3:E:133:LEU:HD22	3:E:225:PRO:HG3	2.01	0.43
1:C:25:LEU:HG	2:D:210:LYS:HD2	2.00	0.43
1:A:120:LYS:HZ2	1:A:124:ARG:NH1	2.17	0.43
2:B:225:GLU:OE1	2:B:226:VAL:HG23	2.18	0.43
2:D:64:VAL:HA	2:D:117:LEU:CD2	2.49	0.43
1:A:71:LEU:HD22	1:A:79:ARG:HG2	2.01	0.43
3:E:208:LEU:HD22	3:E:214:TYR:CZ	2.54	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.74	0.42
3:E:121:SER:O	3:E:122:LYS:O	2.36	0.42
1:A:151:LYS:HB2	1:A:151:LYS:HE2	1.75	0.42
2:B:134:GLN:HG3	2:B:134:GLN:O	2.19	0.42
3:E:130:TYR:HA	3:E:131:PRO:HD2	1.90	0.42
3:E:39:LYS:N	3:E:121:SER:HB2	2.34	0.42
3:R:74:PHE:CD2	3:R:75:ILE:N	2.87	0.42
3:R:142:VAL:CG2	3:R:235:GLN:HB2	2.50	0.42
3:E:101:THR:HA	3:E:108:TYR:CZ	2.54	0.42
1:A:26:LYS:HG2	1:A:39:LEU:HD22	2.01	0.42
1:C:43:ARG:HG2	1:C:169:LEU:HD13	2.02	0.42
2:B:201:TYR:CD2	2:B:201:TYR:N	2.87	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.82	0.42
3:E:50:MET:CE	3:E:131:PRO:HB2	2.49	0.42
2:D:58:ILE:HG12	2:D:58:ILE:H	1.67	0.42
2:B:134:GLN:NE2	2:D:134:GLN:HE21	2.18	0.42
3:E:60:GLU:HA	3:E:60:GLU:OE2	2.20	0.42
3:E:68:THR:HG23	3:E:90:ILE:C	2.40	0.42
3:R:64:GLY:O	3:R:66:LYS:N	2.52	0.42
3:R:63:GLN:O	3:R:64:GLY:C	2.58	0.42
3:R:167:ASP:O	3:R:169:PRO:HD3	2.20	0.42
3:R:41:ALA:O	3:R:42:ASN:HB2	2.20	0.41
2:B:90:SER:O	2:B:91:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH1	1:A:120:LYS:NZ	2.67	0.41
1:A:152:LEU:N	1:A:152:LEU:CD1	2.82	0.41
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.86	0.41
3:E:171:SER:C	3:E:173:GLN:H	2.23	0.41
3:E:177:SER:HA	5:E:402:HOH:O	2.19	0.41
1:C:166:ASP:N	1:C:166:ASP:OD1	2.54	0.41
3:R:190:SER:CB	3:R:192:ARG:HG3	2.48	0.41
3:E:63:GLN:CG	3:E:64:GLY:N	2.83	0.41
1:A:107:ARG:HG2	2:B:84:ILE:HG21	2.03	0.41
3:E:141:GLU:CG	3:E:156:THR:OG1	2.69	0.41
3:R:122:LYS:HB2	3:R:123:TRP:H	1.57	0.41
3:E:68:THR:CG2	3:E:90:ILE:N	2.84	0.41
2:D:168:ALA:HB3	2:D:204:LYS:HG3	2.02	0.41
3:E:81:TRP:O	3:E:82:LEU:HD23	2.20	0.41
3:R:141:GLU:HG3	3:R:156:THR:OG1	2.20	0.41
3:E:57:THR:HA	3:E:58:PRO:HD2	1.84	0.41
2:B:169:TYR:HA	2:B:202:CYS:O	2.21	0.41
3:R:59:PRO:HB2	3:R:60:GLU:H	1.69	0.41
3:E:209:GLU:HA	3:E:210:PRO:HD3	1.84	0.41
3:R:70:THR:HG22	3:R:89:ASN:N	2.34	0.41
3:E:122:LYS:HB2	3:E:123:TRP:H	1.67	0.41
3:R:213:LEU:HD11	3:R:236:CYS:HB3	2.02	0.40
3:E:136:GLN:NE2	3:E:228:ARG:HD3	2.34	0.40
3:E:188:THR:OG1	3:E:213:LEU:HB3	2.21	0.40
3:R:147:ASP:HB3	3:R:150:SER:O	2.21	0.40
2:D:127:LEU:HD21	2:D:129:HIS:O	2.21	0.40
3:R:63:GLN:C	3:R:65:VAL:N	2.73	0.40
2:B:181:LYS:HE2	2:B:181:LYS:HB2	1.86	0.40
1:C:39:LEU:HA	1:C:39:LEU:HD12	1.75	0.40
2:B:35:LEU:HD23	2:B:36:PRO:HD2	2.03	0.40
3:R:104:TYR:N	3:R:104:TYR:CD1	2.87	0.40
3:R:79:LYS:HE3	3:R:79:LYS:HB2	1.84	0.40
2:D:225:GLU:OE1	2:D:226:VAL:N	2.55	0.40
1:C:136:GLU:HG3	1:C:137:GLU:N	2.37	0.40
2:D:143:MET:HG3	2:D:154:ILE:HD11	2.03	0.40
2:D:168:ALA:O	2:D:203:VAL:HA	2.22	0.40
3:E:60:GLU:O	3:E:60:GLU:HG3	2.22	0.40
1:C:102:ASP:OD1	1:C:104:TYR:HB3	2.21	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	151/153 (99%)	141 (93%)	8 (5%)	2 (1%)	15	44
1	C	151/153 (99%)	142 (94%)	7 (5%)	2 (1%)	15	44
2	B	191/206 (93%)	174 (91%)	14 (7%)	3 (2%)	12	38
2	D	191/206 (93%)	173 (91%)	13 (7%)	5 (3%)	7	22
3	E	202/221 (91%)	178 (88%)	18 (9%)	6 (3%)	5	18
3	R	202/221 (91%)	184 (91%)	14 (7%)	4 (2%)	9	30
All	All	1088/1160 (94%)	992 (91%)	74 (7%)	22 (2%)	9	30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	59	PRO
3	R	122	LYS
1	C	67	ARG
3	E	59	PRO
3	E	122	LYS
1	A	67	ARG
1	A	154	PRO
2	B	118	GLY
3	R	64	GLY
2	D	118	GLY
2	D	200	ALA
3	E	64	GLY
1	C	154	PRO
2	D	91	LEU
3	E	89	ASN
2	B	62	GLU
2	B	200	ALA
3	R	89	ASN
2	D	40	GLN
3	E	231	PRO

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Mol	Chain	Res	Type
2	D	38	PRO
3	E	58	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	137/137 (100%)	121 (88%)	16 (12%)	7 20
1	C	137/137 (100%)	123 (90%)	14 (10%)	9 26
2	B	168/177 (95%)	152 (90%)	16 (10%)	11 30
2	D	168/177 (95%)	147 (88%)	21 (12%)	6 17
3	E	186/201 (92%)	163 (88%)	23 (12%)	6 17
3	R	186/201 (92%)	164 (88%)	22 (12%)	6 19
All	All	982/1030 (95%)	870 (89%)	112 (11%)	7 21

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	39	LEU
1	A	60	ILE
1	A	71	LEU
1	A	72	GLN
1	A	82	LEU
1	A	88	ARG
1	A	93	ARG
1	A	106	LEU
1	A	124	ARG
1	A	132	CYS
1	A	147	SER
1	A	151	LYS
1	A	152	LEU
1	A	168	LEU
1	A	176	GLU

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Mol	Chain	Res	Type
2	B	35	LEU
2	B	46	THR
2	B	58	ILE
2	B	63	THR
2	B	91	LEU
2	B	114	ARG
2	B	120	GLN
2	B	139	THR
2	B	147	LYS
2	B	177	GLU
2	B	180	VAL
2	B	181	LYS
2	B	182	MET
2	B	184	ARG
2	B	222	GLU
2	B	225	GLU
3	R	48	ILE
3	R	71	VAL
3	R	88	ARG
3	R	89	ASN
3	R	92	ARG
3	R	107	GLN
3	R	119	LYS
3	R	122	LYS
3	R	123	TRP
3	R	130	TYR
3	R	142	VAL
3	R	145	THR
3	R	155	LEU
3	R	159	GLU
3	R	163	ARG
3	R	168	LEU
3	R	184	SER
3	R	192	ARG
3	R	202	THR
3	R	233	GLU
3	R	234	LYS
3	R	235	GLN
1	C	29	ASN
1	C	39	LEU
1	C	50	ARG
1	C	52	SER

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Mol	Chain	Res	Type
1	C	71	LEU
1	C	82	LEU
1	C	88	ARG
1	C	93	ARG
1	C	106	LEU
1	C	124	ARG
1	C	151	LYS
1	C	152	LEU
1	C	168	LEU
1	C	176	GLU
2	D	35	LEU
2	D	44	LEU
2	D	49	LYS
2	D	52	LEU
2	D	58	ILE
2	D	63	THR
2	D	97	CYS
2	D	114	ARG
2	D	120	GLN
2	D	125	SER
2	D	139	THR
2	D	140	ARG
2	D	145	ILE
2	D	177	GLU
2	D	180	VAL
2	D	181	LYS
2	D	182	MET
2	D	184	ARG
2	D	203	VAL
2	D	222	GLU
2	D	225	GLU
3	E	43	ILE
3	E	48	ILE
3	E	71	VAL
3	E	88	ARG
3	E	104	TYR
3	E	122	LYS
3	E	130	TYR
3	E	142	VAL
3	E	155	LEU
3	E	159	GLU
3	E	168	LEU

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Mol	Chain	Res	Type
3	E	170	VAL
3	E	184	SER
3	E	192	ARG
3	E	195	SER
3	E	200	ASN
3	E	202	THR
3	E	220	SER
3	E	221	PHE
3	E	232	SER
3	E	233	GLU
3	E	234	LYS
3	E	235	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	72	GLN
1	A	78	ASN
1	A	144	GLN
2	B	47	ASN
2	B	110	ASN
2	B	120	GLN
2	B	134	GLN
2	B	206	GLN
3	R	42	ASN
3	R	52	ASN
3	R	55	GLN
3	R	63	GLN
3	R	89	ASN
3	R	136	GLN
3	R	235	GLN
1	C	29	ASN
1	C	40	GLN
1	C	54	GLN
2	D	110	ASN
2	D	120	GLN
2	D	134	GLN
2	D	206	GLN
3	E	42	ASN
3	E	52	ASN
3	E	63	GLN

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Mol	Chain	Res	Type
3	E	89	ASN
3	E	106	HIS
3	E	136	GLN
3	E	211	ASN
3	E	235	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)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	301	-	14,14,15	0.81	0	15,19,21	1.37	2 (13%)
4	NAG	D	301	-	14,14,15	0.53	0	15,19,21	2.22	3 (20%)
4	NAG	E	301	-	14,14,15	1.63	2 (14%)	15,19,21	2.08	2 (13%)
4	NAG	R	301	-	14,14,15	0.58	0	15,19,21	1.34	2 (13%)
4	NAG	R	302	-	14,14,15	0.67	0	15,19,21	1.37	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
4	NAG	B	301	-	-	0/6/23/26	0/1/1/1
4	NAG	D	301	-	-	0/6/23/26	0/1/1/1
4	NAG	E	301	-	-	0/6/23/26	0/1/1/1
4	NAG	R	301	-	-	0/6/23/26	0/1/1/1
4	NAG	R	302	-	-	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)
4	E	301	NAG	O5-C1	-5.01	1.35	1.43
4	E	301	NAG	C1-C2	-2.25	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	NAG	C2-N2-C7	-6.71	114.41	123.04
4	E	301	NAG	C1-O5-C5	-5.83	104.85	112.25
4	R	301	NAG	C2-N2-C7	-2.52	119.80	123.04
4	B	301	NAG	O7-C7-C8	-2.38	117.69	122.06
4	D	301	NAG	O4-C4-C3	-2.21	105.36	110.34
4	B	301	NAG	C1-O5-C5	2.27	115.13	112.25
4	D	301	NAG	C1-O5-C5	2.64	115.60	112.25
4	R	301	NAG	C3-C4-C5	3.27	115.91	110.20
4	R	302	NAG	C3-C4-C5	3.58	116.44	110.20
4	E	301	NAG	C3-C4-C5	4.54	118.11	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	NAG	2	0
4	D	301	NAG	1	0
4	E	301	NAG	4	0
4	R	301	NAG	2	0
4	R	302	NAG	7	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	153/153 (100%)	-0.21	1 (0%) 89 84	28, 48, 72, 104	0
1	C	153/153 (100%)	-0.30	0 100 100	27, 49, 73, 102	0
2	B	193/206 (93%)	-0.03	2 (1%) 84 77	34, 55, 93, 110	0
2	D	193/206 (93%)	0.22	11 (5%) 27 17	34, 55, 98, 116	0
3	E	204/221 (92%)	0.22	12 (5%) 26 16	41, 67, 114, 134	0
3	R	204/221 (92%)	0.22	9 (4%) 38 26	40, 66, 112, 133	0
All	All	1100/1160 (94%)	0.04	35 (3%) 51 39	27, 57, 101, 134	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	62	GLU	6.7
2	D	117	LEU	6.5
3	R	66	LYS	6.1
3	E	65	VAL	5.4
3	E	62	LEU	5.4
1	A	176	GLU	5.1
2	D	59	ALA	4.4
3	E	148	GLU	4.1
2	D	116	THR	3.9
3	R	115	ILE	3.9
3	R	116	TRP	3.9
3	E	63	GLN	3.6
2	D	60	PRO	3.4
3	R	62	LEU	3.4
2	D	61	GLY	3.4
3	R	120	CYS	3.3
3	E	66	LYS	3.2
3	E	61	GLY	3.2
3	R	63	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
3	R	117	GLY	2.8
3	E	116	TRP	2.8
2	D	93	GLU	2.7
2	D	199	ALA	2.7
3	E	229	ALA	2.5
2	D	118	GLY	2.5
3	R	65	VAL	2.4
3	E	230	GLN	2.3
2	B	174	PRO	2.3
3	E	168	LEU	2.3
3	R	88	ARG	2.3
3	E	232	SER	2.2
2	D	225	GLU	2.2
2	B	117	LEU	2.1
3	E	207	TRP	2.0
2	D	65	TYR	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 (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	R	302	14/15	0.84	0.27	2.23	49,51,54,54	0
4	NAG	E	301	14/15	0.85	0.23	1.92	49,51,54,54	0
4	NAG	D	301	14/15	0.87	0.37	-	54,58,61,64	0
4	NAG	B	301	14/15	0.79	0.37	-	54,58,61,64	0
4	NAG	R	301	14/15	0.81	0.29	-	49,51,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.