



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VT4
Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MUTATIONS AND BOUND CYANOPINDOLOL
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Deposited on : 2008-05-09
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

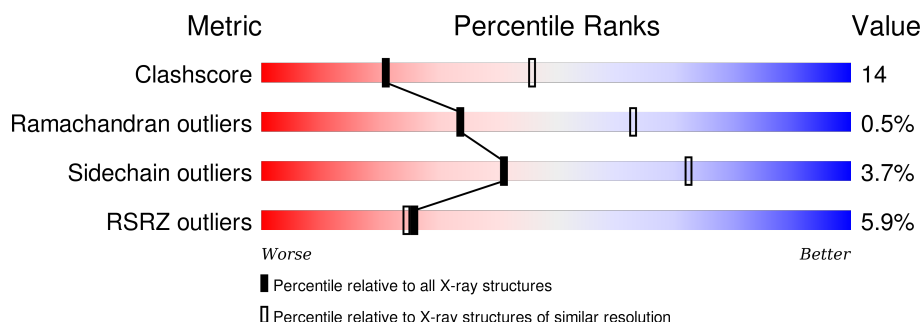
1 Overall quality at a glance

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))
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 $\leq 5\%$. 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	313	
1	B	313	
1	C	313	
1	D	313	

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	SOG	A	402	-	-	-	X
4	SOG	A	405	-	-	-	X
4	SOG	B	402	-	-	-	X
4	SOG	B	404	-	-	-	X
4	SOG	C	404	-	-	-	X
4	SOG	C	405	-	-	-	X
4	SOG	D	402	-	-	-	X
4	SOG	D	405	-	-	-	X
5	D10	A	406	-	-	-	X
5	D10	C	406	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8976 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 BETA1 ADRENERGIC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2175	1441	355	361	18			
1	B	276	Total	C	N	O	S	0	0	0
			2195	1455	358	364	18			
1	C	263	Total	C	N	O	S	0	0	0
			2081	1377	337	349	18			
1	D	272	Total	C	N	O	S	0	0	0
			2156	1427	352	359	18			

There are 32 discrepancies between the modelled and reference sequences:

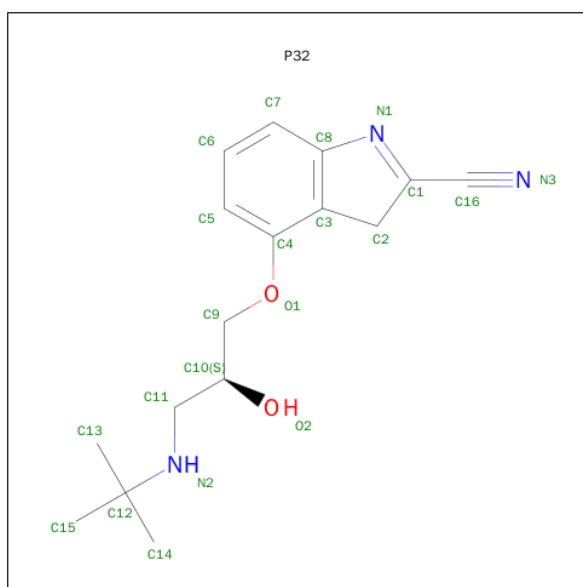
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
A	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
A	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
A	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
A	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700
A	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
A	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
A	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700
B	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
B	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
B	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
B	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
B	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700
B	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
B	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
B	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700
C	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
C	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
C	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
C	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
C	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700

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Chain	Residue	Modelled	Actual	Comment	Reference
C	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
C	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
C	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700
D	68	SER	ARG	ENGINEERED MUTATION	UNP P07700
D	90	VAL	MET	ENGINEERED MUTATION	UNP P07700
D	116	LEU	CYS	ENGINEERED MUTATION	UNP P07700
D	227	ALA	TYR	ENGINEERED MUTATION	UNP P07700
D	282	LEU	ALA	ENGINEERED MUTATION	UNP P07700
D	327	ALA	PHE	ENGINEERED MUTATION	UNP P07700
D	338	MET	PHE	ENGINEERED MUTATION	UNP P07700
D	358	ALA	CYS	ENGINEERED MUTATION	UNP P07700

- Molecule 2 is 4-[(2S)-3-(TERT-BUTYLAMINO)-2-HYDROXYPROPYL]OXY}-3H-INDOLE-2-CARBONITRILE (three-letter code: P32) (formula: C₁₆H₂₁N₃O₂).

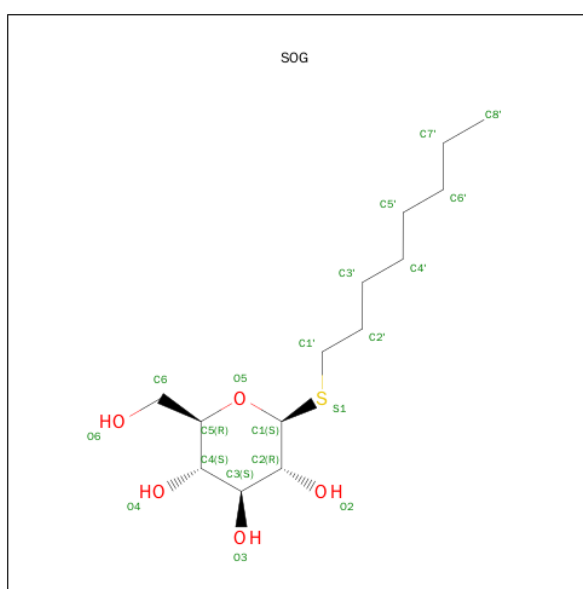


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	16	3	2		
2	B	1	Total	C	N	O	0	0
			21	16	3	2		
2	C	1	Total	C	N	O	0	0
			21	16	3	2		
2	D	1	Total	C	N	O	0	0
			21	16	3	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is SUGAR (2-HYDROXYMETHYL-6-OCTYLSULFANYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: SOG) (formula: C₁₄H₂₈O₅S).



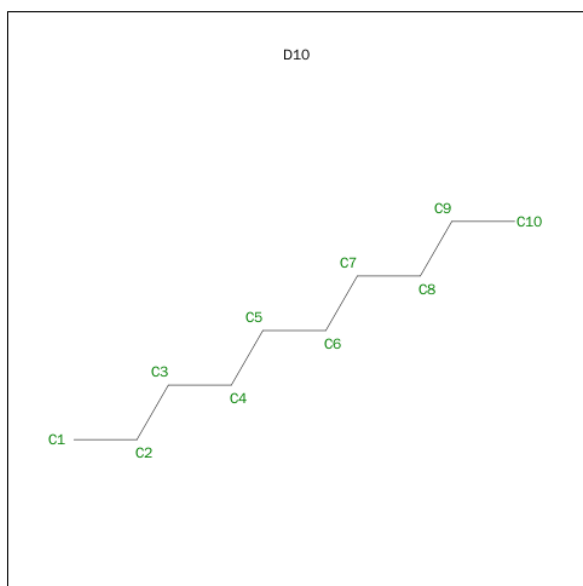
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C O S 20 14 5 1	0	0
4	B	1	Total C O S 20 14 5 1	0	0
4	B	1	Total C S 10 9 1	0	0
4	B	1	Total C O S 20 14 5 1	0	0
4	C	1	Total C O S 20 14 5 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O S 20 14 5 1	0	0
4	C	1	Total C O S 20 14 5 1	0	0
4	D	1	Total C O S 20 14 5 1	0	0
4	D	1	Total C O S 20 14 5 1	0	0
4	D	1	Total C O S 20 14 5 1	0	0

- Molecule 5 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 10 10	0	0
5	C	1	Total C 10 10	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	7	Total O 7 7	0	0

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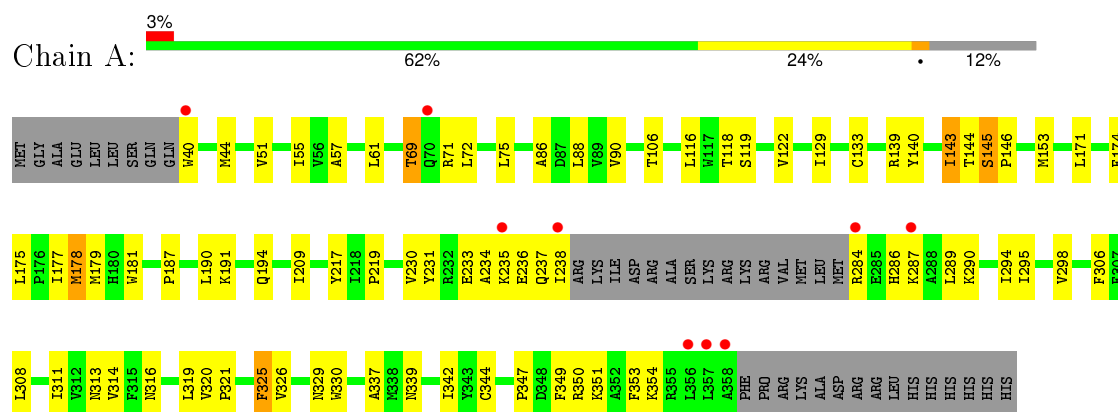
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	7	Total	O	0	0
			7	7		
6	D	8	Total	O	0	0
			8	8		

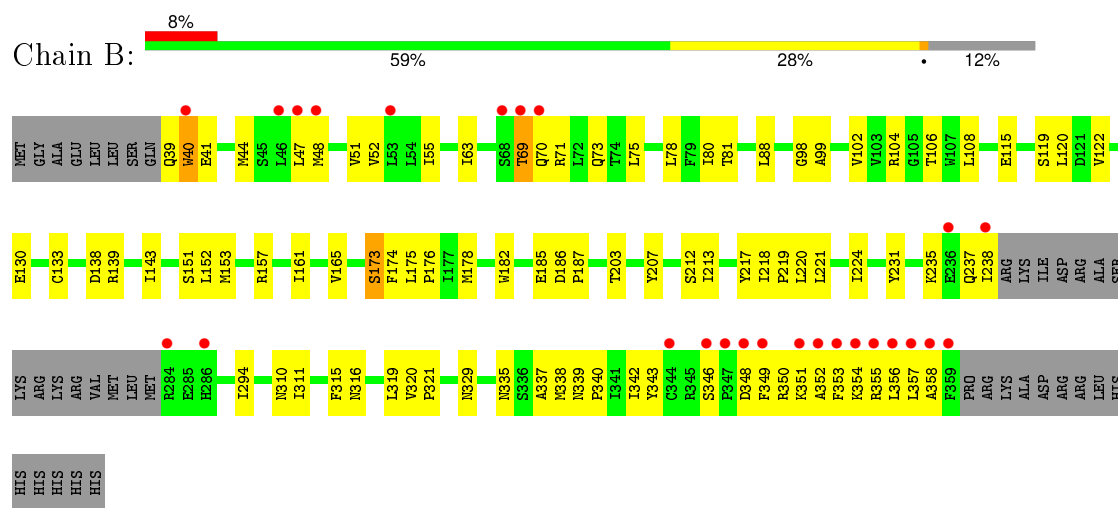
3 Residue-property plots

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.

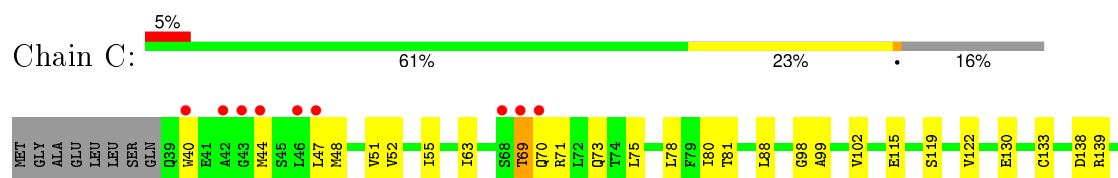
• Molecule 1: BETA1 ADRENERGIC RECEPTOR

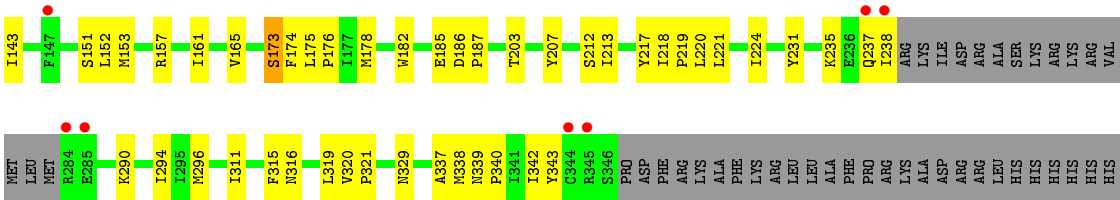


• Molecule 1: BETA1 ADRENERGIC RECEPTOR

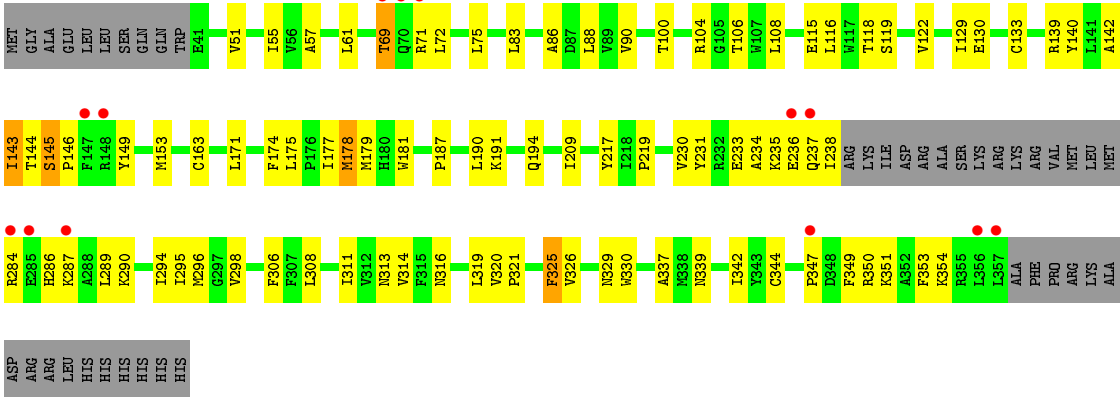


• Molecule 1: BETA1 ADRENERGIC RECEPTOR





• Molecule 1: BETA1 ADRENERGIC RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.50Å 86.80Å 95.50Å 67.60° 73.30° 85.80°	Depositor
Resolution (Å)	45.10 – 2.70 45.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.10-2.70) 83.6 (45.14-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.PHASER)	Depositor
R, R_{free}	0.212 , 0.268 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 41499 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: P32, NA, D10, SOG

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	0.47	1/2229 (0.0%)	0.58	0/3042
1	B	0.46	0/2250	0.58	1/3070 (0.0%)
1	C	0.44	0/2132	0.58	0/2913
1	D	0.46	0/2208	0.59	0/3012
All	All	0.46	1/8819 (0.0%)	0.58	1/12037 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	CYS	CB-SG	-6.39	1.71	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2250	64	0
1	B	2195	0	2267	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2081	0	2145	59	0
1	D	2156	0	2235	71	0
2	A	21	0	21	0	0
2	B	21	0	21	2	0
2	C	21	0	21	1	0
2	D	21	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	60	0	83	7	0
4	B	50	0	73	5	0
4	C	60	0	84	11	0
4	D	60	0	84	9	0
5	A	10	0	22	0	0
5	C	10	0	22	0	0
6	A	9	0	0	0	0
6	B	7	0	0	1	0
6	C	7	0	0	0	0
6	D	8	0	0	0	0
All	All	8976	0	9349	262	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 14.

All (262) 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:290:LYS:HA	4:C:405:SOG:H2'1	1.47	0.95
1:D:104:ARG:HG2	1:D:108:LEU:HD11	1.58	0.84
1:C:122:VAL:HG12	1:C:173:SER:HB2	1.64	0.80
1:D:238:ILE:HB	1:D:286:HIS:CE1	2.16	0.80
1:B:122:VAL:HG12	1:B:173:SER:HB2	1.65	0.78
1:D:295:ILE:HD12	1:D:339:ASN:ND2	2.00	0.77
1:D:313:ASN:ND2	1:D:325:PHE:HE1	1.81	0.77
1:C:290:LYS:HG3	4:C:405:SOG:H1'2	1.66	0.76
1:A:295:ILE:HD12	1:A:339:ASN:ND2	2.02	0.75
1:A:313:ASN:ND2	1:A:325:PHE:HE1	1.84	0.74
1:D:235:LYS:HD3	1:D:236:GLU:OE2	1.88	0.74
1:B:346:SER:O	1:B:350:ARG:HB2	1.89	0.72
1:A:235:LYS:O	1:A:238:ILE:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLY:O	1:C:102:VAL:HG23	1.93	0.69
1:B:98:GLY:O	1:B:102:VAL:HG23	1.95	0.67
1:A:69:THR:HG22	1:A:71:ARG:HB3	1.75	0.67
1:A:233:GLU:O	1:A:237:GLN:HB2	1.95	0.67
1:D:69:THR:HG22	1:D:71:ARG:HB3	1.75	0.67
1:D:233:GLU:O	1:D:237:GLN:HB2	1.95	0.67
1:B:106:THR:HG21	4:D:403:SOG:H1	1.78	0.66
1:B:70:GLN:HA	1:B:73:GLN:HB2	1.77	0.65
1:A:71:ARG:HH22	1:A:351:LYS:NZ	1.96	0.64
1:D:129:ILE:HG13	1:D:219:PRO:HB2	1.78	0.64
1:D:71:ARG:HH22	1:D:351:LYS:NZ	1.96	0.64
1:C:70:GLN:HA	1:C:73:GLN:HB2	1.77	0.64
1:B:231:TYR:CD1	4:B:405:SOG:H3'1	2.33	0.63
1:A:129:ILE:HG13	1:A:219:PRO:HB2	1.79	0.63
1:B:157:ARG:HG2	4:B:404:SOG:H2'1	1.80	0.62
1:D:313:ASN:ND2	1:D:325:PHE:CE1	2.65	0.62
1:D:178:MET:HA	4:D:403:SOG:C1'	2.28	0.62
1:B:316:ASN:ND2	1:B:319:LEU:HB2	2.14	0.62
4:A:402:SOG:H2'2	4:A:402:SOG:O5	2.00	0.62
1:C:316:ASN:ND2	1:C:319:LEU:HB2	2.15	0.62
1:D:296:MET:SD	4:D:405:SOG:H8'3	2.40	0.62
1:C:48:MET:HG2	1:C:99:ALA:HB1	1.81	0.61
1:B:48:MET:HG2	1:B:99:ALA:HB1	1.80	0.61
1:D:234:ALA:O	1:D:286:HIS:HE1	1.84	0.61
1:C:217:TYR:CE1	1:C:311:ILE:HD11	2.36	0.61
1:A:313:ASN:ND2	1:A:325:PHE:CE1	2.67	0.61
1:B:186:ASP:OD1	1:B:187:PRO:HD2	2.02	0.60
1:C:186:ASP:OD1	1:C:187:PRO:HD2	2.02	0.60
1:B:217:TYR:CE1	1:B:311:ILE:HD11	2.36	0.60
1:D:55:ILE:HG13	1:D:337:ALA:HB2	1.83	0.60
1:B:294:ILE:HG22	1:B:342:ILE:HD13	1.83	0.60
1:A:55:ILE:HG13	1:A:337:ALA:HB2	1.83	0.60
1:C:218:ILE:HB	1:C:219:PRO:HD3	1.83	0.59
1:B:346:SER:HB3	1:B:349:PHE:HB2	1.85	0.59
1:A:235:LYS:C	1:A:237:GLN:H	2.04	0.59
1:B:161:ILE:HG12	4:B:404:SOG:H6'1	1.84	0.59
1:B:218:ILE:HB	1:B:219:PRO:HD3	1.83	0.59
1:C:161:ILE:HG12	4:C:404:SOG:H6'1	1.85	0.59
1:B:213:ILE:HA	1:B:217:TYR:HB2	1.84	0.58
1:C:294:ILE:HG22	1:C:342:ILE:HD13	1.85	0.58
1:A:234:ALA:O	1:A:286:HIS:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:HA	1:C:217:TYR:HB2	1.84	0.57
1:A:289:LEU:O	4:A:405:SOG:H3'2	2.05	0.57
1:B:231:TYR:HD1	4:B:405:SOG:H3'1	1.69	0.57
1:C:231:TYR:HD1	4:C:405:SOG:H3'1	1.68	0.57
1:B:350:ARG:HG2	1:B:354:LYS:NZ	2.20	0.56
1:D:290:LYS:HG3	4:D:405:SOG:S1	2.45	0.56
1:B:185:GLU:OE1	1:B:185:GLU:HA	2.05	0.56
1:A:116:LEU:O	1:A:119:SER:HB2	2.05	0.56
1:D:349:PHE:HB3	1:D:353:PHE:CE2	2.41	0.56
1:B:335:ASN:ND2	6:B:2007:HOH:O	2.22	0.56
1:A:294:ILE:HG22	1:A:342:ILE:HD13	1.87	0.55
1:A:143:ILE:O	1:A:143:ILE:HG23	2.06	0.55
1:D:116:LEU:O	1:D:119:SER:HB2	2.07	0.55
1:B:353:PHE:O	1:B:357:LEU:HD12	2.07	0.55
1:C:185:GLU:HA	1:C:185:GLU:OE1	2.07	0.55
1:B:338:MET:O	1:B:342:ILE:HG13	2.07	0.54
1:D:238:ILE:HB	1:D:286:HIS:HE1	1.70	0.54
1:A:349:PHE:HB3	1:A:353:PHE:CE2	2.42	0.54
1:A:181:TRP:CD1	4:A:402:SOG:O6	2.61	0.54
1:D:209:ILE:HD11	1:D:314:VAL:HG11	1.88	0.54
1:D:234:ALA:O	1:D:286:HIS:CE1	2.60	0.54
1:A:140:TYR:HB2	1:A:230:VAL:CG2	2.38	0.54
1:C:122:VAL:HG12	1:C:173:SER:CB	2.37	0.54
1:D:143:ILE:HG23	1:D:143:ILE:O	2.07	0.54
1:D:140:TYR:HB2	1:D:230:VAL:CG2	2.39	0.53
1:A:71:ARG:O	1:A:71:ARG:HG2	2.07	0.53
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.89	0.53
1:D:294:ILE:HG22	1:D:342:ILE:HD13	1.89	0.53
1:A:40:TRP:O	1:A:44:MET:HG2	2.09	0.53
1:C:338:MET:O	1:C:342:ILE:HG13	2.09	0.52
1:C:235:LYS:O	1:C:238:ILE:HG22	2.09	0.52
1:C:339:ASN:HB2	1:C:340:PRO:HD3	1.90	0.52
1:C:48:MET:O	1:C:51:VAL:HG22	2.09	0.52
1:B:122:VAL:HG12	1:B:173:SER:CB	2.38	0.52
1:A:284:ARG:HD3	1:A:287:LYS:HD2	1.91	0.52
1:A:234:ALA:O	1:A:286:HIS:CE1	2.63	0.52
1:A:347:PRO:O	1:A:351:LYS:HG3	2.10	0.52
1:C:115:GLU:HB3	1:C:178:MET:HE3	1.90	0.52
1:D:284:ARG:HD3	1:D:287:LYS:HD2	1.91	0.52
1:C:75:LEU:O	1:C:78:LEU:HB2	2.10	0.52
1:B:119:SER:HB3	1:B:174:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:O	1:A:330:TRP:HD1	1.93	0.52
1:D:326:VAL:O	1:D:330:TRP:HD1	1.93	0.52
1:B:48:MET:HG2	1:B:99:ALA:CB	2.40	0.51
1:C:119:SER:HB3	1:C:174:PHE:CD2	2.45	0.51
1:A:75:LEU:HD13	1:A:153:MET:CG	2.40	0.51
1:A:231:TYR:HD1	4:A:405:SOG:H1'1	1.75	0.51
1:D:71:ARG:HG2	1:D:71:ARG:O	2.09	0.51
1:B:235:LYS:O	1:B:238:ILE:HG22	2.10	0.51
1:B:339:ASN:HB2	1:B:340:PRO:HD3	1.91	0.51
1:A:171:LEU:HD12	1:A:175:LEU:HD12	1.92	0.51
1:D:75:LEU:HD13	1:D:153:MET:CG	2.40	0.51
1:B:119:SER:HB3	1:B:174:PHE:CE2	2.46	0.51
1:D:171:LEU:HD12	1:D:175:LEU:HD12	1.92	0.51
1:C:48:MET:HG2	1:C:99:ALA:CB	2.41	0.50
1:B:182:TRP:O	1:B:203:THR:HA	2.11	0.50
1:C:182:TRP:O	1:C:203:THR:HA	2.12	0.50
1:B:48:MET:O	1:B:51:VAL:HG22	2.10	0.50
1:A:118:THR:O	1:A:122:VAL:HG23	2.10	0.50
1:D:235:LYS:C	1:D:237:GLN:H	2.13	0.50
1:C:115:GLU:HB3	1:C:178:MET:CE	2.42	0.50
1:D:347:PRO:O	1:D:351:LYS:HG3	2.12	0.50
1:C:119:SER:HB3	1:C:174:PHE:CE2	2.46	0.50
1:A:316:ASN:HB3	1:A:319:LEU:HB2	1.92	0.50
1:D:316:ASN:HB3	1:D:319:LEU:HB2	1.92	0.50
1:C:231:TYR:CD1	4:C:405:SOG:H3'1	2.47	0.50
1:D:71:ARG:HH22	1:D:351:LYS:HZ2	1.58	0.49
1:D:118:THR:O	1:D:122:VAL:HG23	2.11	0.49
1:A:295:ILE:HD12	1:A:339:ASN:CG	2.33	0.49
1:C:319:LEU:O	1:C:319:LEU:HG	2.13	0.49
1:B:152:LEU:O	1:B:157:ARG:NH1	2.40	0.49
1:B:115:GLU:HB3	1:B:178:MET:HE3	1.93	0.49
1:D:295:ILE:HD12	1:D:339:ASN:CG	2.33	0.49
4:A:405:SOG:H3'2	4:A:405:SOG:H6'1	1.53	0.49
1:B:319:LEU:HG	1:B:319:LEU:O	2.13	0.49
1:C:207:TYR:C	1:C:207:TYR:CD2	2.86	0.49
1:B:351:LYS:O	1:B:355:ARG:HG3	2.13	0.49
1:B:75:LEU:HD13	1:B:153:MET:HG3	1.94	0.49
1:B:75:LEU:O	1:B:78:LEU:HB2	2.13	0.49
1:C:152:LEU:O	1:C:157:ARG:NH1	2.42	0.48
1:B:207:TYR:C	1:B:207:TYR:CD2	2.86	0.48
1:D:178:MET:HB2	4:D:403:SOG:O6	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD13	1:C:153:MET:HG3	1.94	0.48
1:B:104:ARG:HH22	1:D:115:GLU:CD	2.17	0.48
1:A:174:PHE:O	1:A:178:MET:HG2	2.12	0.48
1:A:290:LYS:HA	4:A:405:SOG:H2'1	1.95	0.48
1:B:115:GLU:HB3	1:B:178:MET:CE	2.44	0.48
1:D:145:SER:N	1:D:146:PRO:CD	2.76	0.48
1:C:55:ILE:HG12	1:C:337:ALA:HB2	1.96	0.48
1:C:130:GLU:HB3	1:C:165:VAL:HG13	1.95	0.48
1:D:86:ALA:O	1:D:90:VAL:HG23	2.13	0.48
1:A:139:ARG:NE	1:A:139:ARG:HA	2.28	0.48
1:D:174:PHE:O	1:D:178:MET:HG2	2.13	0.48
1:C:122:VAL:HG13	2:C:400:P32:C6	2.44	0.47
1:B:55:ILE:HG12	1:B:337:ALA:HB2	1.96	0.47
1:A:71:ARG:HH22	1:A:351:LYS:HZ2	1.59	0.47
1:D:71:ARG:HH12	1:D:351:LYS:NZ	2.11	0.47
1:A:71:ARG:HH12	1:A:351:LYS:NZ	2.12	0.47
1:A:86:ALA:O	1:A:90:VAL:HG23	2.14	0.47
1:D:57:ALA:O	1:D:61:LEU:HB2	2.15	0.47
1:D:75:LEU:HD13	1:D:153:MET:HG2	1.96	0.47
1:D:231:TYR:HD1	4:D:405:SOG:H3'1	1.79	0.47
1:A:145:SER:N	1:A:146:PRO:CD	2.78	0.47
1:B:130:GLU:HB3	1:B:165:VAL:HG13	1.96	0.47
1:D:217:TYR:CE1	1:D:311:ILE:HD11	2.50	0.47
1:D:139:ARG:HA	1:D:139:ARG:NE	2.29	0.47
1:B:69:THR:HG22	1:B:71:ARG:HB3	1.96	0.47
1:B:217:TYR:O	1:B:221:LEU:HG	2.15	0.46
1:C:51:VAL:HG23	1:C:52:VAL:N	2.31	0.46
1:B:122:VAL:HG13	2:B:400:P32:C6	2.44	0.46
1:C:217:TYR:O	1:C:221:LEU:HG	2.15	0.46
1:B:63:ILE:HG12	1:B:81:THR:HG23	1.97	0.46
1:C:44:MET:O	1:C:48:MET:HB2	2.16	0.46
1:B:51:VAL:HG23	1:B:52:VAL:N	2.31	0.46
1:A:143:ILE:HG22	1:A:144:THR:HG23	1.96	0.46
1:A:187:PRO:O	1:A:191:LYS:HG3	2.15	0.46
1:D:289:LEU:O	4:D:405:SOG:H4'1	2.15	0.46
1:A:75:LEU:HD13	1:A:153:MET:HG2	1.97	0.46
1:A:57:ALA:O	1:A:61:LEU:HB2	2.15	0.46
1:C:69:THR:HG22	1:C:71:ARG:HB3	1.97	0.46
1:A:238:ILE:HG23	1:A:286:HIS:HE1	1.82	0.45
1:D:143:ILE:HG22	1:D:144:THR:HG23	1.98	0.45
1:B:120:LEU:HA	1:B:120:LEU:HD23	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HG12	1:C:81:THR:HG23	1.98	0.45
4:C:402:SOG:O6	1:D:163:CYS:HB3	2.16	0.45
1:A:238:ILE:HD13	4:A:405:SOG:O3	2.17	0.45
1:B:44:MET:O	1:B:48:MET:HB2	2.17	0.45
1:A:217:TYR:CE1	1:A:311:ILE:HD11	2.52	0.44
1:C:290:LYS:CA	4:C:405:SOG:H2'1	2.33	0.44
1:D:178:MET:HA	4:D:403:SOG:H1'1	1.96	0.44
1:A:235:LYS:O	1:A:237:GLN:N	2.51	0.44
1:C:157:ARG:HG2	4:C:404:SOG:H2'1	1.99	0.44
1:D:69:THR:HB	1:D:72:LEU:HB2	2.00	0.44
1:A:344:CYS:O	1:A:350:ARG:HD3	2.18	0.44
1:C:290:LYS:HG3	4:C:405:SOG:C1'	2.44	0.44
1:D:100:THR:O	1:D:104:ARG:HB3	2.18	0.44
1:D:235:LYS:C	1:D:237:GLN:N	2.70	0.44
1:D:235:LYS:O	1:D:237:GLN:N	2.51	0.44
1:B:352:ALA:O	1:B:356:LEU:HD12	2.18	0.44
1:B:69:THR:CG2	1:B:71:ARG:HB3	2.48	0.44
1:D:179:MET:HE2	1:D:181:TRP:NE1	2.32	0.44
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.73	0.44
1:A:320:VAL:HA	1:A:321:PRO:HD3	1.78	0.44
1:A:294:ILE:O	1:A:298:VAL:HG23	2.19	0.43
1:D:344:CYS:O	1:D:350:ARG:HD3	2.19	0.43
1:A:235:LYS:C	1:A:237:GLN:N	2.70	0.43
1:C:55:ILE:CG1	1:C:337:ALA:HB2	2.48	0.43
1:D:143:ILE:CG2	1:D:144:THR:HG23	2.49	0.43
1:D:306:PHE:C	1:D:306:PHE:CD2	2.92	0.43
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.69	0.43
1:C:296:MET:HE1	4:C:405:SOG:C8'	2.49	0.43
1:A:306:PHE:CD2	1:A:306:PHE:C	2.92	0.43
1:A:69:THR:HB	1:A:72:LEU:HB2	2.01	0.43
1:C:69:THR:CG2	1:C:71:ARG:HB3	2.49	0.43
1:D:179:MET:HE2	1:D:181:TRP:HE1	1.83	0.43
1:B:315:PHE:N	1:B:315:PHE:CD1	2.86	0.43
1:B:39:GLN:C	1:B:41:GLU:N	2.72	0.43
1:B:122:VAL:CG1	1:B:173:SER:HB2	2.44	0.42
1:D:187:PRO:O	1:D:191:LYS:HG3	2.17	0.42
1:B:310:ASN:HD21	2:B:400:P32:C16	2.31	0.42
1:A:129:ILE:O	1:A:129:ILE:HD12	2.19	0.42
1:C:40:TRP:CE2	1:C:44:MET:HE3	2.55	0.42
1:B:75:LEU:CD1	1:B:153:MET:HG3	2.49	0.42
1:B:55:ILE:CG1	1:B:337:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HD12	1:B:343:TYR:OH	2.20	0.42
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.83	0.42
1:C:296:MET:CE	4:C:405:SOG:C8'	2.97	0.42
1:D:294:ILE:O	1:D:298:VAL:HG23	2.20	0.42
1:B:235:LYS:C	1:B:237:GLN:H	2.23	0.42
1:B:220:LEU:HG	1:B:224:ILE:HD12	2.00	0.42
1:C:80:ILE:HD12	1:C:343:TYR:OH	2.20	0.42
1:A:179:MET:HE2	1:A:181:TRP:NE1	2.33	0.42
1:C:152:LEU:HD23	1:C:152:LEU:HA	1.83	0.42
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.69	0.42
1:B:320:VAL:HG13	1:B:321:PRO:HD2	2.00	0.42
1:A:143:ILE:CG2	1:A:144:THR:HG23	2.49	0.42
1:C:235:LYS:C	1:C:237:GLN:H	2.23	0.42
1:A:75:LEU:HD13	1:A:153:MET:HG3	2.01	0.42
1:D:350:ARG:O	1:D:354:LYS:HG3	2.19	0.42
1:B:175:LEU:HB2	1:B:176:PRO:HD3	2.01	0.42
1:D:320:VAL:HA	1:D:321:PRO:HD3	1.79	0.42
1:A:350:ARG:O	1:A:354:LYS:HG3	2.19	0.41
1:C:315:PHE:N	1:C:315:PHE:CD1	2.87	0.41
1:C:75:LEU:CD1	1:C:153:MET:HG3	2.50	0.41
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.75	0.41
1:C:220:LEU:HG	1:C:224:ILE:HD12	2.02	0.41
1:B:40:TRP:CE2	1:B:44:MET:HE3	2.56	0.41
1:A:119:SER:HB3	1:A:174:PHE:CE2	2.56	0.41
1:C:139:ARG:NE	1:C:139:ARG:HA	2.35	0.41
1:D:190:LEU:O	1:D:194:GLN:HG2	2.21	0.41
1:B:231:TYR:CE1	4:B:405:SOG:H3'1	2.55	0.41
1:A:179:MET:HE2	1:A:181:TRP:HE1	1.85	0.41
1:A:140:TYR:HB2	1:A:230:VAL:HG22	2.02	0.41
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.93	0.41
1:C:339:ASN:CB	1:C:340:PRO:HD3	2.51	0.41
1:C:175:LEU:HB2	1:C:176:PRO:HD3	2.02	0.41
1:D:238:ILE:HD12	1:D:286:HIS:ND1	2.36	0.41
1:D:296:MET:CE	4:D:405:SOG:C8'	2.98	0.41
1:C:88:LEU:HD12	1:C:88:LEU:HA	1.93	0.41
1:A:238:ILE:HG23	1:A:286:HIS:CE1	2.56	0.40
1:D:129:ILE:O	1:D:129:ILE:HD12	2.20	0.40
1:D:142:ALA:HB2	1:D:149:TYR:CE1	2.56	0.40
1:B:139:ARG:HA	1:B:139:ARG:NE	2.36	0.40
1:A:190:LEU:O	1:A:194:GLN:HG2	2.21	0.40
1:D:130:GLU:O	1:D:133:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LEU:HD12	1:D:83:LEU:HA	1.85	0.40
1:B:339:ASN:CB	1:B:340:PRO:HD3	2.52	0.40
1:C:320:VAL:HG13	1:C:321:PRO:HD2	2.02	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	270/313 (86%)	258 (96%)	10 (4%)	2 (1%)	26	55
1	B	272/313 (87%)	249 (92%)	21 (8%)	2 (1%)	26	55
1	C	259/313 (83%)	241 (93%)	18 (7%)	0	100	100
1	D	268/313 (86%)	254 (95%)	13 (5%)	1 (0%)	39	69
All	All	1069/1252 (85%)	1002 (94%)	62 (6%)	5 (0%)	34	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	B	40	TRP
1	A	69	THR
1	D	69	THR
1	B	358	ALA

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	236/271 (87%)	228 (97%)	8 (3%)	44	75
1	B	238/271 (88%)	228 (96%)	10 (4%)	36	68
1	C	227/271 (84%)	218 (96%)	9 (4%)	38	69
1	D	235/271 (87%)	227 (97%)	8 (3%)	44	75
All	All	936/1084 (86%)	901 (96%)	35 (4%)	41	72

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	106	THR
1	A	143	ILE
1	A	145	SER
1	A	177	ILE
1	A	178	MET
1	A	325	PHE
1	A	329	ASN
1	B	47	LEU
1	B	69	THR
1	B	133	CYS
1	B	138	ASP
1	B	143	ILE
1	B	151	SER
1	B	173	SER
1	B	212	SER
1	B	329	ASN
1	B	348	ASP
1	C	47	LEU
1	C	69	THR
1	C	133	CYS
1	C	138	ASP
1	C	143	ILE
1	C	151	SER
1	C	173	SER
1	C	212	SER
1	C	329	ASN
1	D	51	VAL
1	D	106	THR
1	D	143	ILE

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Mol	Chain	Res	Type
1	D	145	SER
1	D	177	ILE
1	D	178	MET
1	D	325	PHE
1	D	329	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	313	ASN
1	B	310	ASN
1	C	310	ASN
1	D	286	HIS
1	D	313	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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
2	P32	A	400	-	21,22,22	2.47	2 (9%)	26,31,31	1.57	4 (15%)
4	SOG	A	402	-	20,20,20	1.86	6 (30%)	23,25,25	2.41	8 (34%)
4	SOG	A	403	-	20,20,20	0.59	0	23,25,25	0.91	0
4	SOG	A	405	-	20,20,20	1.01	2 (10%)	23,25,25	1.12	2 (8%)
5	D10	A	406	-	9,9,9	0.63	0	8,8,8	0.57	0
2	P32	B	400	-	21,22,22	2.48	2 (9%)	26,31,31	1.89	4 (15%)
4	SOG	B	402	-	20,20,20	0.89	1 (5%)	23,25,25	2.03	3 (13%)
4	SOG	B	404	-	9,9,20	0.60	0	8,8,25	1.16	1 (12%)
4	SOG	B	405	-	20,20,20	0.79	1 (5%)	23,25,25	0.86	1 (4%)
2	P32	C	400	-	21,22,22	2.46	2 (9%)	26,31,31	1.96	5 (19%)
4	SOG	C	402	-	20,20,20	0.70	1 (5%)	23,25,25	1.82	2 (8%)
4	SOG	C	404	-	20,20,20	0.89	1 (5%)	23,25,25	1.15	2 (8%)
4	SOG	C	405	-	20,20,20	0.65	0	23,25,25	1.61	3 (13%)
5	D10	C	406	-	9,9,9	0.57	0	8,8,8	0.64	0
2	P32	D	400	-	21,22,22	2.52	2 (9%)	26,31,31	1.63	5 (19%)
4	SOG	D	402	-	20,20,20	1.20	2 (10%)	23,25,25	1.55	2 (8%)
4	SOG	D	403	-	20,20,20	0.61	0	23,25,25	2.31	7 (30%)
4	SOG	D	405	-	20,20,20	0.54	0	23,25,25	0.97	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
2	P32	A	400	-	-	0/11/21/21	0/2/2/2
4	SOG	A	402	-	-	0/11/31/31	0/1/1/1
4	SOG	A	403	-	-	0/11/31/31	0/1/1/1
4	SOG	A	405	-	-	0/11/31/31	0/1/1/1
5	D10	A	406	-	-	0/7/7/7	0/0/0/0
2	P32	B	400	-	-	0/11/21/21	0/2/2/2
4	SOG	B	402	-	-	0/11/31/31	0/1/1/1
4	SOG	B	404	-	-	0/7/7/31	0/0/0/1
4	SOG	B	405	-	-	0/11/31/31	0/1/1/1
2	P32	C	400	-	-	0/11/21/21	0/2/2/2
4	SOG	C	402	-	-	0/11/31/31	0/1/1/1
4	SOG	C	404	-	-	0/11/31/31	0/1/1/1
4	SOG	C	405	-	-	0/11/31/31	0/1/1/1
5	D10	C	406	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P32	D	400	-	-	0/11/21/21	0/2/2/2
4	SOG	D	402	-	-	0/11/31/31	0/1/1/1
4	SOG	D	403	-	-	0/11/31/31	0/1/1/1
4	SOG	D	405	-	-	0/11/31/31	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	P32	C2-C3	-10.61	1.32	1.51
2	B	400	P32	C2-C3	-10.40	1.32	1.51
2	A	400	P32	C2-C3	-10.29	1.33	1.51
2	C	400	P32	C2-C3	-10.02	1.33	1.51
2	A	400	P32	C8-N1	-3.35	1.33	1.39
2	D	400	P32	C8-N1	-3.20	1.33	1.39
2	C	400	P32	C8-N1	-3.11	1.33	1.39
2	B	400	P32	C8-N1	-2.95	1.34	1.39
4	A	402	SOG	C4-C5	2.09	1.57	1.53
4	B	405	SOG	C1-S1	2.09	1.84	1.80
4	D	402	SOG	C1-S1	2.15	1.84	1.80
4	A	402	SOG	C6-C5	2.16	1.59	1.51
4	C	404	SOG	O5-C1	2.17	1.46	1.42
4	A	402	SOG	C1'-S1	2.18	1.84	1.81
4	C	402	SOG	O5-C1	2.19	1.46	1.42
4	A	405	SOG	O5-C1	2.37	1.46	1.42
4	A	405	SOG	C1-S1	2.55	1.84	1.80
4	D	402	SOG	O5-C1	2.60	1.46	1.42
4	B	402	SOG	O5-C1	2.75	1.47	1.42
4	A	402	SOG	O5-C5	3.26	1.52	1.44
4	A	402	SOG	C1-S1	3.74	1.86	1.80
4	A	402	SOG	O5-C1	5.09	1.51	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	P32	C11-N2-C12	-7.23	108.76	116.50
2	B	400	P32	C11-N2-C12	-6.68	109.35	116.50
4	D	403	SOG	O5-C5-C6	-6.40	90.18	106.36
4	B	402	SOG	C6-C5-C4	-6.08	98.03	113.02
4	C	405	SOG	C1'-S1-C1	-5.89	92.17	100.30
4	D	403	SOG	C6-C5-C4	-5.04	100.58	113.02
2	B	400	P32	C3-C8-N1	-4.39	106.74	111.86
2	C	400	P32	C3-C8-N1	-4.26	106.88	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	P32	C11-N2-C12	-4.21	112.00	116.50
2	A	400	P32	C3-C8-N1	-4.19	106.97	111.86
2	D	400	P32	C3-C8-N1	-4.13	107.04	111.86
4	C	402	SOG	C6-C5-C4	-4.13	102.83	113.02
2	A	400	P32	C11-N2-C12	-3.75	112.48	116.50
4	D	403	SOG	C1-O5-C5	-3.30	106.44	112.74
4	D	403	SOG	C1-C2-C3	-3.24	103.51	110.69
2	A	400	P32	C11-C10-C9	-2.48	106.15	110.43
4	D	403	SOG	O4-C4-C3	-2.35	105.04	110.34
4	C	405	SOG	C6'-C5'-C4'	-2.35	102.39	114.53
2	C	400	P32	O1-C4-C5	-2.21	119.38	124.01
4	B	404	SOG	C3'-C2'-C1'	-2.20	104.08	113.18
2	D	400	P32	C11-C10-C9	-2.18	106.66	110.43
4	C	405	SOG	C4'-C3'-C2'	-2.14	103.50	114.53
2	B	400	P32	O1-C4-C5	-2.12	119.57	124.01
4	D	403	SOG	C1'-S1-C1	-2.11	97.39	100.30
4	A	405	SOG	C5'-C4'-C3'	-2.10	103.69	114.53
4	A	402	SOG	C3-C4-C5	-2.04	106.64	110.20
2	D	400	P32	O1-C4-C3	2.03	119.14	115.83
4	A	402	SOG	O4-C4-C5	2.11	114.84	109.24
2	A	400	P32	O1-C4-C3	2.15	119.34	115.83
2	C	400	P32	C3-C2-C1	2.16	106.55	102.86
4	B	402	SOG	O5-C5-C6	2.22	111.97	106.36
2	B	400	P32	O1-C4-C3	2.34	119.65	115.83
2	C	400	P32	O1-C4-C3	2.38	119.71	115.83
4	A	402	SOG	O2-C2-C1	2.46	115.22	110.43
4	C	404	SOG	O5-C5-C6	2.46	112.57	106.36
2	D	400	P32	C3-C2-C1	2.47	107.09	102.86
4	B	405	SOG	O5-C5-C6	2.56	112.82	106.36
4	D	402	SOG	O5-C5-C6	2.71	113.20	106.36
4	D	403	SOG	O5-C1-C2	2.78	113.96	110.19
4	C	404	SOG	C1'-S1-C1	2.81	104.17	100.30
4	A	402	SOG	C4'-C3'-C2'	3.13	130.69	114.53
4	A	402	SOG	O5-C1-S1	3.30	118.33	109.85
4	A	405	SOG	O5-C5-C6	3.32	114.75	106.36
4	A	402	SOG	C6-C5-C4	3.37	121.32	113.02
4	D	402	SOG	C6-C5-C4	4.41	123.89	113.02
4	A	402	SOG	C1'-S1-C1	4.98	107.17	100.30
4	B	402	SOG	C1'-S1-C1	5.59	108.00	100.30
4	C	402	SOG	C1'-S1-C1	6.25	108.92	100.30
4	A	402	SOG	O5-C5-C6	6.85	123.67	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	SOG	2	0
4	A	405	SOG	5	0
2	B	400	P32	2	0
4	B	404	SOG	2	0
4	B	405	SOG	3	0
2	C	400	P32	1	0
4	C	402	SOG	1	0
4	C	404	SOG	2	0
4	C	405	SOG	8	0
4	D	403	SOG	4	0
4	D	405	SOG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	274/313 (87%)	-0.04	9 (3%)	50	50	19, 36, 82, 119	0
1	B	276/313 (88%)	0.26	26 (9%)	11	8	21, 41, 104, 138	0
1	C	263/313 (84%)	-0.02	16 (6%)	25	23	21, 40, 87, 120	0
1	D	272/313 (86%)	-0.10	13 (4%)	34	33	20, 36, 81, 119	0
All	All	1085/1252 (86%)	0.03	64 (5%)	26	24	19, 38, 88, 138	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	PHE	8.0
1	B	358	ALA	7.9
1	B	352	ALA	7.7
1	B	353	PHE	7.3
1	B	347	PRO	5.9
1	B	348	ASP	5.6
1	B	354	LYS	5.4
1	D	356	LEU	5.4
1	B	349	PHE	5.3
1	A	284	ARG	5.0
1	B	355	ARG	4.8
1	D	284	ARG	4.3
1	D	237	GLN	4.2
1	D	357	LEU	4.1
1	C	44	MET	4.1
1	C	238	ILE	4.0
1	A	238	ILE	3.9
1	C	147	PHE	3.8
1	B	351	LYS	3.8
1	B	357	LEU	3.7
1	B	70	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	40	TRP	3.7
1	C	40	TRP	3.6
1	A	356	LEU	3.5
1	B	356	LEU	3.5
1	B	238	ILE	3.4
1	C	284	ARG	3.3
1	B	344	CYS	3.2
1	B	284	ARG	3.2
1	A	70	GLN	3.1
1	D	69	THR	3.0
1	C	46	LEU	3.0
1	D	287	LYS	2.9
1	B	47	LEU	2.9
1	C	70	GLN	2.8
1	D	236	GLU	2.8
1	D	70	GLN	2.8
1	B	53	LEU	2.8
1	C	47	LEU	2.8
1	B	48	MET	2.8
1	B	68	SER	2.8
1	D	285	GLU	2.7
1	A	235	LYS	2.6
1	B	346	SER	2.6
1	B	46	LEU	2.6
1	C	344	CYS	2.5
1	D	71	ARG	2.5
1	A	357	LEU	2.4
1	C	43	GLY	2.4
1	A	358	ALA	2.4
1	C	68	SER	2.4
1	C	42	ALA	2.3
1	C	69	THR	2.3
1	B	69	THR	2.3
1	D	347	PRO	2.3
1	C	237	GLN	2.2
1	B	286	HIS	2.2
1	B	236	GLU	2.1
1	A	287	LYS	2.1
1	B	40	TRP	2.1
1	C	285	GLU	2.1
1	D	147	PHE	2.1
1	C	345	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	148	ARG	2.1

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, 95th 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	D10	C	406	10/10	0.81	0.32	7.86	36,49,60,60	0
5	D10	A	406	10/10	0.92	0.35	4.96	25,41,47,48	0
4	SOG	C	404	20/20	0.80	0.25	4.75	29,95,123,123	0
4	SOG	D	405	20/20	0.72	0.45	3.79	41,115,131,133	0
4	SOG	A	402	20/20	0.80	0.27	3.60	33,54,74,94	0
4	SOG	D	402	20/20	0.81	0.25	3.60	26,54,88,90	0
4	SOG	B	404	10/20	0.91	0.23	3.45	30,42,48,81	0
4	SOG	C	405	20/20	0.67	0.46	2.53	55,107,126,128	0
4	SOG	A	405	20/20	0.79	0.48	2.44	39,89,110,116	0
4	SOG	B	402	20/20	0.82	0.23	2.17	19,90,122,125	0
4	SOG	D	403	20/20	0.92	0.17	1.69	18,36,54,72	0
4	SOG	C	402	20/20	0.83	0.20	1.62	18,91,111,113	0
4	SOG	B	405	20/20	0.68	0.31	1.45	55,114,128,131	0
2	P32	B	400	21/21	0.97	0.16	0.52	19,33,39,50	0
3	NA	B	401	1/1	0.83	0.15	0.36	40,40,40,40	0
2	P32	A	400	21/21	0.96	0.17	0.17	17,32,41,44	0
2	P32	C	400	21/21	0.97	0.15	0.03	22,33,43,51	0
3	NA	C	401	1/1	0.93	0.14	-0.03	36,36,36,36	0
2	P32	D	400	21/21	0.97	0.16	-0.03	17,33,40,42	0
4	SOG	A	403	20/20	0.95	0.14	-0.72	28,39,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	A	401	1/1	0.98	0.08	-0.97	33,33,33,33	0
3	NA	D	401	1/1	0.88	0.08	-1.33	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.