



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:26 PM UTC

PDB ID : 5K5S / pdb_00005k5s
Title : Crystal structure of the active form of human calcium-sensing receptor extra-cellular domain
Authors : Geng, Y.; Mosyak, L.; Kurinov, I.; Zuo, H.; Sturchler, E.; Cheng, T.C.; Subramanyam, P.; Brown, A.P.; Brennan, S.C.; Mun, H.-C.; Bush, M.; Chen, Y.; Nguyen, T.; Cao, B.; Chang, D.; Quick, M.; Conigrave, A.; Colecraft, H.M.; McDonald, P.; Fan, Q.R.
Deposited on : 2016-05-23
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

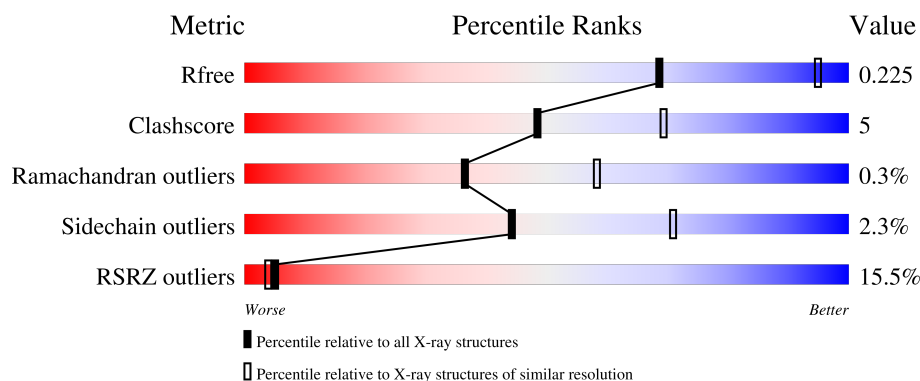
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	615	
1	B	615	

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:

Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	702	-	X	-	-
3	PO4	B	703	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8913 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 Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4203	2675	707	800	21			
1	B	537	Total	C	N	O	S	0	0	0
			4251	2703	717	810	21			

There are 60 discrepancies between the modelled and reference sequences:

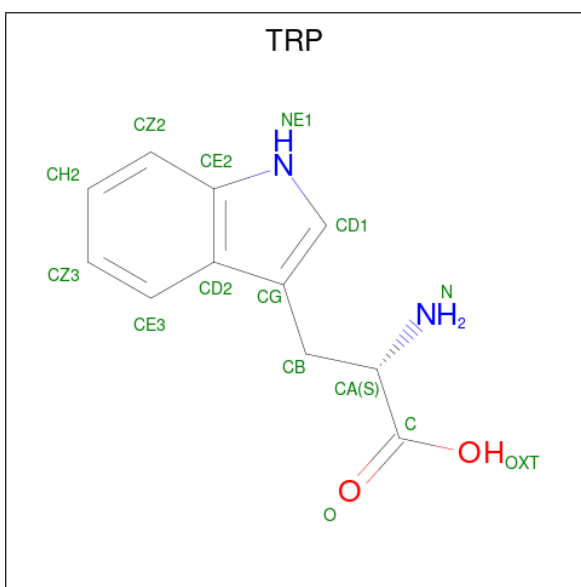
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P41180
A	2	ALA	-	expression tag	UNP P41180
A	3	PHE	-	expression tag	UNP P41180
A	4	TYR	-	expression tag	UNP P41180
A	5	SER	-	expression tag	UNP P41180
A	6	CYS	-	expression tag	UNP P41180
A	7	CYS	-	expression tag	UNP P41180
A	8	TRP	-	expression tag	UNP P41180
A	9	VAL	-	expression tag	UNP P41180
A	10	LEU	-	expression tag	UNP P41180
A	11	LEU	-	expression tag	UNP P41180
A	12	ALA	-	expression tag	UNP P41180
A	13	LEU	-	expression tag	UNP P41180
A	14	THR	-	expression tag	UNP P41180
A	15	TRP	-	expression tag	UNP P41180
A	16	HIS	-	expression tag	UNP P41180
A	17	THR	-	expression tag	UNP P41180
A	18	SER	-	expression tag	UNP P41180
A	19	ALA	-	expression tag	UNP P41180
A	386	GLN	ASN	engineered mutation	UNP P41180
A	402	ASN	SER	engineered mutation	UNP P41180
A	468	GLN	ASN	engineered mutation	UNP P41180
A	608	ASP	-	expression tag	UNP P41180
A	609	TYR	-	expression tag	UNP P41180
A	610	LYS	-	expression tag	UNP P41180

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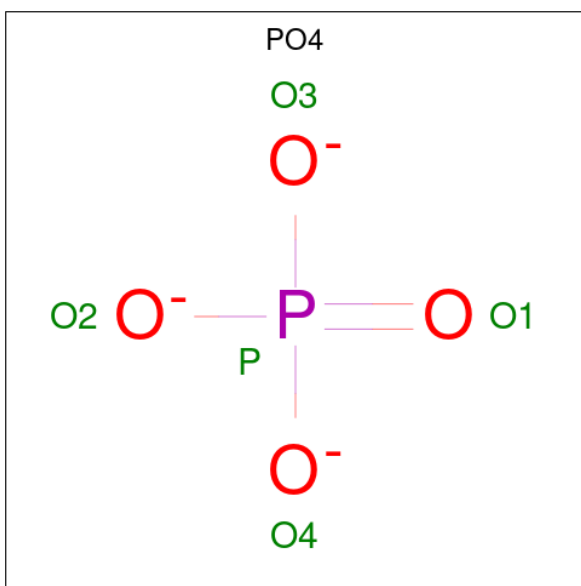
Chain	Residue	Modelled	Actual	Comment	Reference
A	611	ASP	-	expression tag	UNP P41180
A	612	ASP	-	expression tag	UNP P41180
A	613	ASP	-	expression tag	UNP P41180
A	614	ASP	-	expression tag	UNP P41180
A	615	LYS	-	expression tag	UNP P41180
B	1	MET	-	initiating methionine	UNP P41180
B	2	ALA	-	expression tag	UNP P41180
B	3	PHE	-	expression tag	UNP P41180
B	4	TYR	-	expression tag	UNP P41180
B	5	SER	-	expression tag	UNP P41180
B	6	CYS	-	expression tag	UNP P41180
B	7	CYS	-	expression tag	UNP P41180
B	8	TRP	-	expression tag	UNP P41180
B	9	VAL	-	expression tag	UNP P41180
B	10	LEU	-	expression tag	UNP P41180
B	11	LEU	-	expression tag	UNP P41180
B	12	ALA	-	expression tag	UNP P41180
B	13	LEU	-	expression tag	UNP P41180
B	14	THR	-	expression tag	UNP P41180
B	15	TRP	-	expression tag	UNP P41180
B	16	HIS	-	expression tag	UNP P41180
B	17	THR	-	expression tag	UNP P41180
B	18	SER	-	expression tag	UNP P41180
B	19	ALA	-	expression tag	UNP P41180
B	386	GLN	ASN	engineered mutation	UNP P41180
B	402	ASN	SER	engineered mutation	UNP P41180
B	468	GLN	ASN	engineered mutation	UNP P41180
B	608	ASP	-	expression tag	UNP P41180
B	609	TYR	-	expression tag	UNP P41180
B	610	LYS	-	expression tag	UNP P41180
B	611	ASP	-	expression tag	UNP P41180
B	612	ASP	-	expression tag	UNP P41180
B	613	ASP	-	expression tag	UNP P41180
B	614	ASP	-	expression tag	UNP P41180
B	615	LYS	-	expression tag	UNP P41180

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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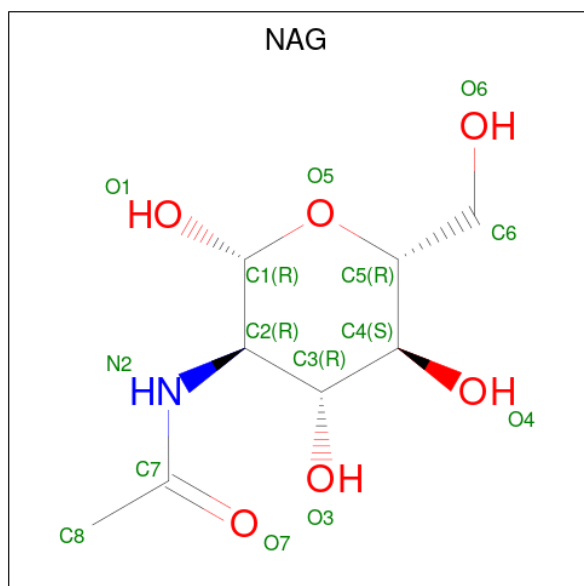
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Ca	0	0
			5	5		
4	B	3	Total	Ca	0	0
			3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

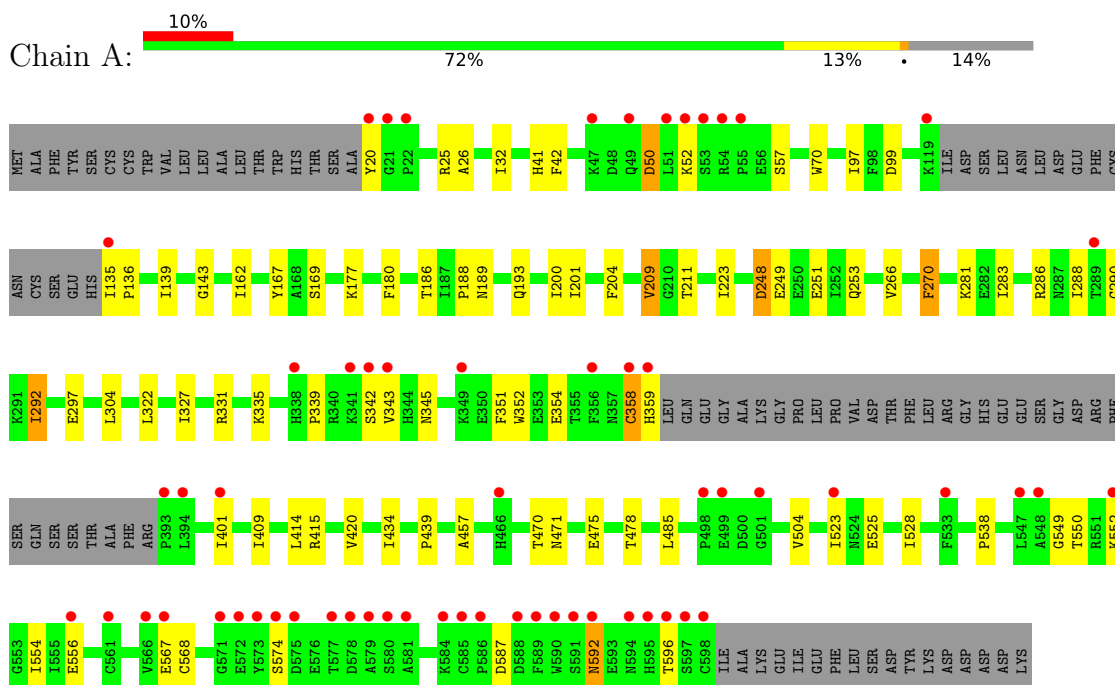
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total 189	O 189	0	0
6	B	142	Total 142	O 142	0	0

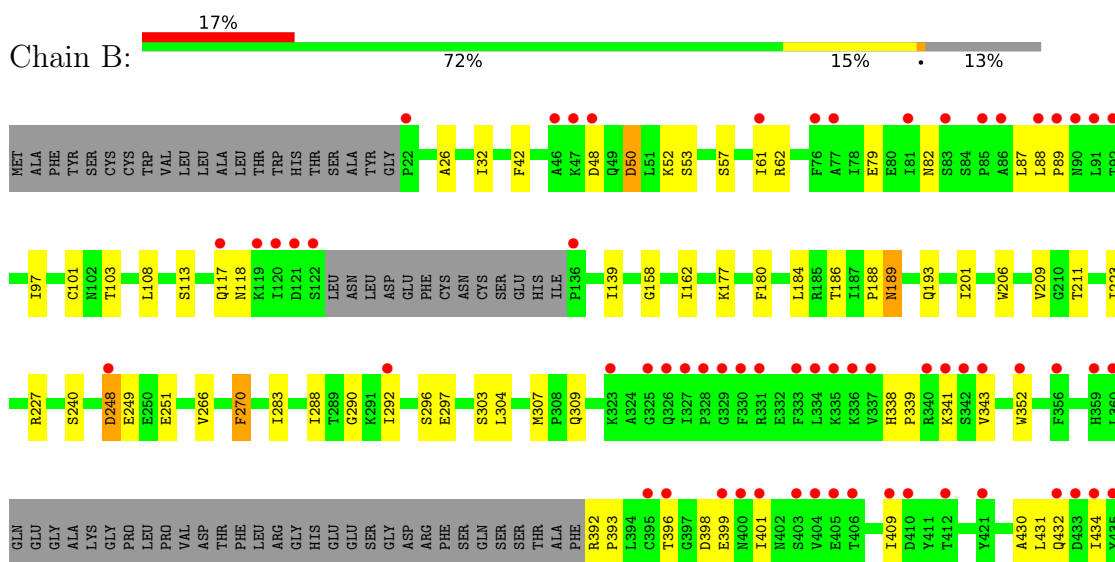
3 Residue-property plots

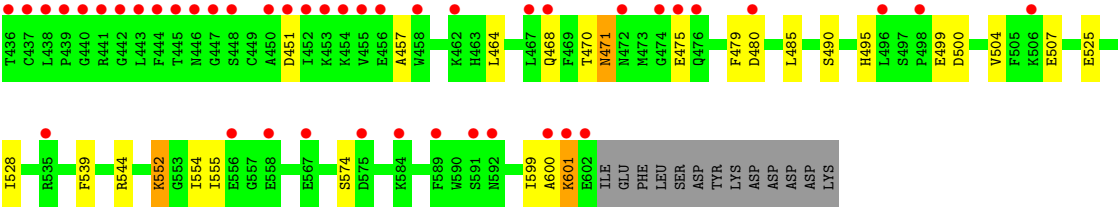
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Extracellular calcium-sensing receptor



- Molecule 1: Extracellular calcium-sensing receptor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.66Å 127.45Å 146.77Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	38.07 – 2.60 38.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.7 (38.07-2.60) 84.7 (38.07-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.211 , 0.222 (Not available) , 0.225	Depositor DCC
R_{free} test set	2476 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8913	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PO4, 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	0/4305	1.35	21/5837 (0.4%)
1	B	0.78	0/4352	1.40	37/5898 (0.6%)
All	All	0.76	0/8657	1.38	58/11735 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ASN	CA-C-N	8.43	132.42	120.28
1	B	471	ASN	C-N-CA	8.43	132.42	120.28
1	B	480	ASP	CA-CB-CG	7.86	120.45	112.60
1	A	290	GLY	CA-C-N	7.35	131.27	120.90
1	A	290	GLY	C-N-CA	7.35	131.27	120.90
1	B	189	ASN	CA-CB-CG	7.24	119.84	112.60
1	B	118	ASN	CA-C-N	7.05	130.67	120.38
1	B	118	ASN	C-N-CA	7.05	130.67	120.38
1	B	290	GLY	CA-C-N	6.73	130.39	120.90
1	B	290	GLY	C-N-CA	6.73	130.39	120.90
1	B	89	PRO	CA-C-N	6.64	129.17	120.28
1	B	89	PRO	C-N-CA	6.64	129.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	343	VAL	N-CA-C	-6.36	103.14	111.09
1	A	249	GLU	N-CA-C	-6.31	104.48	111.36
1	A	50	ASP	N-CA-C	-6.30	105.07	112.89
1	B	471	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	470	THR	CA-C-N	5.98	130.97	120.87
1	A	470	THR	C-N-CA	5.98	130.97	120.87
1	B	479	PHE	CA-C-N	5.96	131.56	120.95
1	B	479	PHE	C-N-CA	5.96	131.56	120.95
1	A	434	ILE	CA-C-N	5.90	128.11	120.44
1	A	434	ILE	C-N-CA	5.90	128.11	120.44
1	B	188	PRO	CA-C-N	5.72	128.99	120.87
1	B	188	PRO	C-N-CA	5.72	128.99	120.87
1	B	470	THR	CA-C-N	5.72	131.12	120.95
1	B	470	THR	C-N-CA	5.72	131.12	120.95
1	B	248	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	574	SER	CA-C-N	5.59	127.77	120.28
1	B	574	SER	C-N-CA	5.59	127.77	120.28
1	A	248	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	451	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	50	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	180	PHE	CA-C-N	5.38	127.48	120.28
1	B	180	PHE	C-N-CA	5.38	127.48	120.28
1	B	249	GLU	N-CA-C	-5.36	105.51	111.36
1	B	48	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	552	LYS	CA-C-N	5.25	126.17	122.33
1	B	552	LYS	C-N-CA	5.25	126.17	122.33
1	B	343	VAL	CA-C-N	5.23	127.72	120.29
1	B	343	VAL	C-N-CA	5.23	127.72	120.29
1	A	188	PRO	CA-C-N	5.21	128.27	120.87
1	A	188	PRO	C-N-CA	5.21	128.27	120.87
1	B	158	GLY	CA-C-N	5.20	127.24	120.28
1	B	158	GLY	C-N-CA	5.20	127.24	120.28
1	A	209	VAL	CA-C-N	5.17	125.59	121.61
1	A	209	VAL	C-N-CA	5.17	125.59	121.61
1	B	555	ILE	CA-C-N	5.13	128.51	120.82
1	B	555	ILE	C-N-CA	5.13	128.51	120.82
1	A	358	CYS	N-CA-C	5.09	117.59	109.81
1	A	180	PHE	CA-C-N	5.07	127.59	120.28
1	A	180	PHE	C-N-CA	5.07	127.59	120.28
1	B	292	ILE	CB-CA-C	5.07	117.58	110.99
1	A	351	PHE	CA-C-N	5.06	127.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	PHE	C-N-CA	5.06	127.02	120.44
1	B	409	ILE	CB-CA-C	5.04	115.50	111.06
1	A	592	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	79	GLU	CB-CG-CD	5.03	121.15	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	GLU	Sidechain
1	B	189	ASN	Sidechain

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	4203	0	4037	47	0
1	B	4251	0	4097	43	0
2	A	15	0	9	3	0
2	B	15	0	9	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	56	0	52	0	0
5	B	14	0	13	0	0
6	A	189	0	0	1	0
6	B	142	0	0	2	0
All	All	8913	0	8217	92	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 5.

All (92) 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:A:253:GLN:HE22	1:A:286:ARG:HH11	0.97	0.96
1:A:193:GLN:HE22	1:A:297:GLU:H	1.20	0.88
1:B:193:GLN:HE22	1:B:297:GLU:H	1.22	0.86
1:A:253:GLN:HE22	1:A:286:ARG:NH1	1.73	0.85
1:A:253:GLN:NE2	1:A:286:ARG:HH11	1.75	0.85
1:A:335:LYS:HA	1:A:401:ILE:HD11	1.60	0.83
1:A:32:ILE:HG23	1:A:139:ILE:HG12	1.66	0.77
2:A:701:TRP:N	2:A:701:TRP:CD1	2.54	0.75
1:B:32:ILE:HG23	1:B:139:ILE:HG12	1.69	0.75
1:A:331:ARG:HH22	1:A:409:ILE:HG23	1.54	0.72
1:A:554:ILE:HD12	1:B:552:LYS:HB3	1.71	0.71
2:A:701:TRP:N	2:A:701:TRP:HD1	1.89	0.69
1:A:20:TYR:HB3	1:A:25:ARG:HH22	1.59	0.68
1:B:338:HIS:HB3	1:B:341:LYS:HB2	1.78	0.66
1:B:227:ARG:NH1	1:B:240:SER:HB3	2.12	0.65
1:A:253:GLN:NE2	1:A:286:ARG:NH1	2.41	0.62
2:B:701:TRP:CD1	2:B:701:TRP:N	2.67	0.62
1:B:209:VAL:HG12	1:B:266:VAL:HB	1.81	0.61
1:B:61:ILE:HG22	1:B:62:ARG:HG3	1.83	0.60
1:B:227:ARG:HH12	1:B:240:SER:HB3	1.64	0.60
1:A:331:ARG:NH2	1:A:409:ILE:HG23	2.15	0.60
1:A:209:VAL:HG12	1:A:266:VAL:HB	1.84	0.60
1:A:41:HIS:HD2	1:A:99:ASP:OD2	1.85	0.59
1:B:186:THR:HA	1:B:485:LEU:HD21	1.83	0.59
1:B:193:GLN:HE22	1:B:297:GLU:N	1.97	0.59
1:B:87:LEU:HA	1:B:432:GLN:OE1	2.02	0.59
1:A:266:VAL:HG22	1:A:292:ILE:HD11	1.84	0.59
1:A:50:ASP:HB2	1:A:52:LYS:HG3	1.85	0.58
1:B:82:ASN:HA	6:B:801:HOH:O	2.04	0.57
1:A:169:SER:HA	2:A:701:TRP:OXT	2.05	0.56
1:A:552:LYS:HB3	1:B:554:ILE:HD12	1.88	0.55
1:A:549:GLY:H	1:A:574:SER:HB3	1.71	0.54
1:B:339:PRO:HD3	1:B:352:TRP:CE2	2.43	0.53
1:A:186:THR:HA	1:A:485:LEU:HD12	1.89	0.53
2:B:701:TRP:N	2:B:701:TRP:HD1	2.06	0.53
1:A:568:CYS:SG	1:A:574:SER:HB2	2.49	0.52
1:A:211:THR:HB	1:A:223:ILE:HD12	1.92	0.52
1:A:193:GLN:HE22	1:A:297:GLU:N	1.99	0.52
1:B:211:THR:HB	1:B:223:ILE:HD12	1.90	0.52
1:A:26:ALA:HB3	1:A:97:ILE:HB	1.93	0.51
1:B:307:MET:HE3	1:B:309:GLN:HE22	1.76	0.50
1:B:50:ASP:HB2	1:B:52:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HD13	1:A:209:VAL:HG11	1.93	0.50
1:B:184:LEU:HD11	1:B:464:LEU:HB3	1.93	0.49
1:A:200:ILE:HG12	1:A:523:ILE:HD11	1.93	0.49
1:B:600:ALA:O	1:B:601:LYS:HB2	2.13	0.49
1:B:26:ALA:HB3	1:B:97:ILE:HB	1.95	0.49
1:B:201:ILE:HD13	1:B:209:VAL:HG11	1.94	0.48
1:B:471:ASN:HB3	1:B:475:GLU:H	1.78	0.48
1:B:396:THR:C	1:B:398:ASP:H	2.22	0.48
1:B:223:ILE:HG12	1:B:270:PHE:HB2	1.95	0.48
1:A:478:THR:O	1:A:485:LEU:HD23	2.14	0.48
1:B:352:TRP:CZ3	1:B:399:GLU:HB2	2.48	0.48
1:B:468:GLN:HB3	6:B:819:HOH:O	2.14	0.48
1:A:292:ILE:HG21	1:A:538:PRO:HG2	1.96	0.47
1:A:550:THR:HG22	1:A:567:GLU:HA	1.95	0.47
1:B:101:CYS:O	1:B:103:THR:HG23	2.15	0.47
1:A:248:ASP:HB2	1:A:251:GLU:H	1.80	0.47
1:B:177:LYS:HA	1:B:177:LYS:HD3	1.71	0.46
1:A:223:ILE:HG12	1:A:270:PHE:HB2	1.97	0.45
1:A:525:GLU:HA	1:A:528:ILE:HD12	1.98	0.45
1:A:283:ILE:HG23	1:A:288:ILE:HB	1.97	0.45
1:B:32:ILE:HD13	1:B:431:LEU:HD22	1.98	0.45
1:B:248:ASP:HB2	1:B:251:GLU:H	1.81	0.45
1:A:471:ASN:HB3	1:A:475:GLU:H	1.82	0.45
1:B:539:PHE:CZ	1:B:544:ARG:HD2	2.51	0.45
1:A:292:ILE:HA	6:A:802:HOH:O	2.17	0.45
1:A:204:PHE:HE1	1:A:525:GLU:HG2	1.83	0.44
1:B:495:HIS:HB2	1:B:504:VAL:HG13	1.99	0.44
1:B:352:TRP:HZ3	1:B:399:GLU:HB2	1.82	0.44
1:A:592:ASN:HD21	1:A:596:THR:HB	1.83	0.44
1:A:135:ILE:N	1:A:136:PRO:CD	2.81	0.43
1:B:42:PHE:CZ	1:B:304:LEU:HD11	2.53	0.43
1:B:283:ILE:HG23	1:B:288:ILE:HB	2.00	0.43
1:A:162:ILE:HA	1:A:457:ALA:HB1	2.00	0.43
1:A:342:SER:HB3	1:A:345:ASN:HB3	1.99	0.43
1:A:253:GLN:CD	1:A:286:ARG:NH1	2.77	0.43
1:B:162:ILE:HA	1:B:457:ALA:HB1	2.00	0.43
1:B:392:ARG:N	1:B:393:PRO:HD2	2.33	0.42
1:A:322:LEU:O	1:A:415:ARG:HD3	2.19	0.42
1:B:525:GLU:HA	1:B:528:ILE:HD12	2.01	0.42
1:B:117:GLN:H	1:B:117:GLN:CD	2.27	0.42
1:B:499:GLU:HG3	1:B:500:ASP:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PRO:HD3	1:A:352:TRP:CD2	2.55	0.42
1:A:42:PHE:CZ	1:A:304:LEU:HD11	2.56	0.41
1:A:253:GLN:OE1	1:A:286:ARG:NH1	2.49	0.41
1:A:143:GLY:HA2	1:A:167:TYR:CE2	2.55	0.41
1:B:490:SER:OG	1:B:507:GLU:HG3	2.21	0.41
1:A:327:ILE:HD12	1:A:414:LEU:HD13	2.02	0.41
1:A:70:TRP:HB3	1:A:420:VAL:HG21	2.04	0.40
1:B:430:ALA:O	1:B:434:ILE:HG12	2.21	0.40
1:B:201:ILE:HG23	1:B:206:TRP:HB2	2.04	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	525/615 (85%)	500 (95%)	23 (4%)	2 (0%)	30	51
1	B	531/615 (86%)	502 (94%)	28 (5%)	1 (0%)	43	66
All	All	1056/1230 (86%)	1002 (95%)	51 (5%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	PRO
1	A	587	ASP
1	B	601	LYS

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	457/531 (86%)	448 (98%)	9 (2%)	48	74
1	B	463/531 (87%)	453 (98%)	10 (2%)	45	72
All	All	920/1062 (87%)	901 (98%)	19 (2%)	44	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	177	LYS
1	A	270	PHE
1	A	281	LYS
1	A	292	ILE
1	A	358	CYS
1	A	359	HIS
1	A	504	VAL
1	A	556	GLU
1	B	53	SER
1	B	57	SER
1	B	88	LEU
1	B	108	LEU
1	B	113	SER
1	B	270	PHE
1	B	296	SER
1	B	303	SER
1	B	401	ILE
1	B	599	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	49	GLN
1	A	72	GLN
1	A	117	GLN
1	A	193	GLN
1	A	344	HIS
1	A	413	HIS
1	B	164	GLN

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	344	HIS
1	B	400	ASN
1	B	402	ASN
1	B	413	HIS
1	B	463	HIS
1	B	466	HIS
1	B	595	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\# Z > 2$
3	PO4	A	702	-	4,4,4	2.02	3 (75%)	6,6,6	0.92	0
5	NAG	A	710	1	14,14,15	0.36	0	17,19,21	1.54	3 (17%)
3	PO4	B	702	-	4,4,4	2.12	3 (75%)	6,6,6	1.10	1 (16%)
5	NAG	A	708	1	14,14,15	0.31	0	17,19,21	0.62	0
3	PO4	B	703	-	4,4,4	2.30	4 (100%)	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	707	1	14,14,15	0.44	0	17,19,21	2.56	3 (17%)
3	PO4	A	703	-	4,4,4	2.23	1 (25%)	6,6,6	0.73	0
5	NAG	A	711	1	14,14,15	0.27	0	17,19,21	1.06	1 (5%)
2	TRP	B	701	-	15,16,16	0.73	0	18,22,22	0.47	0
2	TRP	A	701	-	15,16,16	0.77	1 (6%)	18,22,22	0.53	0
5	NAG	A	709	1	14,14,15	0.28	0	17,19,21	0.94	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	710	1	-	5/6/23/26	0/1/1/1
5	NAG	A	708	1	-	0/6/23/26	0/1/1/1
5	NAG	B	707	1	-	5/6/23/26	0/1/1/1
5	NAG	A	711	1	-	4/6/23/26	0/1/1/1
2	TRP	B	701	-	-	3/8/8/8	0/2/2/2
2	TRP	A	701	-	-	3/8/8/8	0/2/2/2
5	NAG	A	709	1	-	4/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	PO4	P-O1	2.93	1.57	1.50
3	B	703	PO4	P-O1	2.83	1.57	1.50
3	B	702	PO4	P-O3	2.35	1.61	1.54
3	A	702	PO4	P-O2	2.28	1.61	1.54
2	A	701	TRP	OXT-C	-2.26	1.23	1.30
3	B	702	PO4	P-O2	2.26	1.61	1.54
3	A	702	PO4	P-O4	2.24	1.61	1.54
3	A	702	PO4	P-O3	2.22	1.61	1.54
3	B	702	PO4	P-O4	2.15	1.60	1.54
3	B	703	PO4	P-O2	2.12	1.60	1.54
3	B	703	PO4	P-O4	2.09	1.60	1.54
3	B	703	PO4	P-O3	2.05	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	707	NAG	C1-O5-C5	7.42	122.13	112.19
5	B	707	NAG	C1-C2-N2	6.01	119.91	110.43
5	A	710	NAG	C2-N2-C7	3.65	127.80	122.90
5	A	710	NAG	C1-C2-N2	-3.62	104.73	110.43
5	A	711	NAG	C1-C2-N2	-3.60	104.76	110.43
5	B	707	NAG	C2-N2-C7	3.31	127.33	122.90
5	A	709	NAG	O5-C1-C2	-2.72	107.09	111.29
5	A	710	NAG	C1-O5-C5	2.19	115.13	112.19
3	B	702	PO4	O3-P-O2	2.04	114.26	107.91
5	A	709	NAG	C1-C2-N2	-2.03	107.23	110.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TRP	N-CA-CB-CG
5	A	710	NAG	C3-C2-N2-C7
5	A	710	NAG	O7-C7-N2-C2
5	B	707	NAG	C1-C2-N2-C7
5	A	710	NAG	C8-C7-N2-C2
5	A	710	NAG	O5-C5-C6-O6
5	A	709	NAG	C8-C7-N2-C2
5	A	711	NAG	C8-C7-N2-C2
5	A	711	NAG	O7-C7-N2-C2
5	A	710	NAG	C4-C5-C6-O6
5	A	709	NAG	O7-C7-N2-C2
5	B	707	NAG	C8-C7-N2-C2
5	A	709	NAG	O5-C5-C6-O6
5	A	709	NAG	C4-C5-C6-O6
5	B	707	NAG	O7-C7-N2-C2
5	B	707	NAG	C4-C5-C6-O6
5	A	711	NAG	C4-C5-C6-O6
5	A	711	NAG	O5-C5-C6-O6
2	B	701	TRP	CA-CB-CG-CD1
2	B	701	TRP	N-CA-CB-CG
2	B	701	TRP	CA-CB-CG-CD2
5	B	707	NAG	O5-C5-C6-O6
2	A	701	TRP	CA-CB-CG-CD1
2	A	701	TRP	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	TRP	2	0
2	A	701	TRP	3	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	531/615 (86%)	0.45	60 (11%)	10 8	20, 53, 133, 211	0
1	B	537/615 (87%)	0.95	106 (19%)	3 2	31, 69, 119, 157	0
All	All	1068/1230 (86%)	0.70	166 (15%)	5 4	20, 61, 126, 211	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	PRO	6.5
1	A	590	TRP	6.2
1	A	589	PHE	6.0
1	B	48	ASP	5.2
1	A	135	ILE	4.9
1	A	119	LYS	4.8
1	B	436	THR	4.7
1	A	586	PRO	4.7
1	B	435	TYR	4.6
1	B	443	LEU	4.6
1	B	122	SER	4.5
1	B	438	LEU	4.5
1	B	404	VAL	4.4
1	B	439	PRO	4.3
1	B	556	GLU	4.2
1	B	120	ILE	3.9
1	A	51	LEU	3.8
1	B	399	GLU	3.8
1	A	20	TYR	3.8
1	B	401	ILE	3.7
1	A	359	HIS	3.6
1	B	136	PRO	3.6
1	A	584	LYS	3.4
1	A	573	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	598	CYS	3.4
1	B	360	LEU	3.4
1	B	474	GLY	3.4
1	B	447	GLY	3.3
1	A	47	LYS	3.3
1	B	352	TRP	3.3
1	A	591	SER	3.3
1	A	548	ALA	3.3
1	B	591	SER	3.3
1	A	49	GLN	3.2
1	A	53	SER	3.2
1	B	323	LYS	3.2
1	B	328	PRO	3.2
1	B	342	SER	3.2
1	B	450	ALA	3.2
1	B	432	GLN	3.2
1	B	448	SER	3.2
1	A	592	ASN	3.2
1	B	453	LYS	3.1
1	A	466	HIS	3.1
1	B	337	VAL	3.1
1	A	54	ARG	3.1
1	B	47	LYS	3.1
1	B	601	LYS	3.1
1	B	600	ALA	3.1
1	B	592	ASN	3.1
1	A	501	GLY	3.1
1	A	581	ALA	3.1
1	B	441	ARG	3.0
1	A	533	PHE	3.0
1	A	401	ILE	3.0
1	B	444	PHE	3.0
1	A	556	GLU	3.0
1	A	577	THR	3.0
1	B	330	PHE	2.9
1	A	341	LYS	2.9
1	B	498	PRO	2.9
1	B	446	ASN	2.9
1	A	578	ASP	2.9
1	B	451	ASP	2.9
1	B	445	THR	2.9
1	B	468	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	462	LYS	2.9
1	B	335	LYS	2.8
1	B	46	ALA	2.8
1	B	85	PRO	2.8
1	A	566	VAL	2.8
1	B	326	GLN	2.8
1	B	92	THR	2.8
1	B	119	LYS	2.8
1	A	575	ASP	2.8
1	A	289	THR	2.8
1	B	86	ALA	2.8
1	A	498	PRO	2.7
1	A	596	THR	2.7
1	B	602	GLU	2.7
1	B	334	LEU	2.7
1	B	405	GLU	2.7
1	B	341	LYS	2.7
1	A	523	ILE	2.6
1	B	467	LEU	2.6
1	B	434	ILE	2.6
1	A	499	GLU	2.6
1	A	571	GLY	2.6
1	B	584	LYS	2.6
1	A	358	CYS	2.6
1	A	22	PRO	2.6
1	B	480	ASP	2.6
1	A	595	HIS	2.6
1	B	89	PRO	2.5
1	A	394	LEU	2.5
1	B	506	LYS	2.5
1	A	21	GLY	2.5
1	B	343	VAL	2.5
1	A	343	VAL	2.5
1	B	76	PHE	2.5
1	B	400	ASN	2.5
1	B	437	CYS	2.5
1	A	55	PRO	2.5
1	B	81	ILE	2.4
1	A	52	LYS	2.4
1	B	340	ARG	2.4
1	B	292	ILE	2.4
1	B	472	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	410	ASP	2.4
1	B	117	GLN	2.4
1	B	396	THR	2.4
1	A	574	SER	2.4
1	A	588	ASP	2.4
1	B	327	ILE	2.4
1	B	395	CYS	2.4
1	B	440	GLY	2.4
1	A	342	SER	2.3
1	A	597	SER	2.3
1	B	83	SER	2.3
1	B	329	GLY	2.3
1	B	476	GLN	2.3
1	B	333	PHE	2.3
1	B	61	ILE	2.3
1	B	409	ILE	2.3
1	B	454	LYS	2.3
1	B	403	SER	2.3
1	B	22	PRO	2.3
1	B	535	ARG	2.3
1	B	589	PHE	2.3
1	B	77	ALA	2.3
1	B	91	LEU	2.3
1	B	412	THR	2.3
1	B	90	ASN	2.3
1	A	580	SER	2.3
1	A	579	ALA	2.3
1	B	359	HIS	2.3
1	B	406	THR	2.3
1	B	121	ASP	2.2
1	B	433	ASP	2.2
1	B	575	ASP	2.2
1	B	88	LEU	2.2
1	B	421	TYR	2.2
1	B	336	LYS	2.2
1	B	475	GLU	2.2
1	B	496	LEU	2.2
1	B	558	GLU	2.2
1	B	452	ILE	2.2
1	B	455	VAL	2.2
1	B	456	GLU	2.1
1	B	331	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	561	CYS	2.1
1	A	585	CYS	2.1
1	A	594	ASN	2.1
1	A	338	HIS	2.1
1	B	567	GLU	2.1
1	A	567	GLU	2.1
1	A	349	LYS	2.1
1	A	572	GLU	2.1
1	B	458	TRP	2.1
1	B	248	ASP	2.0
1	B	325	GLY	2.0
1	B	442	GLY	2.0
1	A	356	PHE	2.0
1	B	356	PHE	2.0
1	A	552	LYS	2.0
1	A	547	LEU	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	NAG	A	708	14/15	0.52	0.18	88,91,94,95	0
4	CA	A	707	1/1	0.59	0.19	139,139,139,139	0
4	CA	A	712	1/1	0.69	0.20	140,140,140,140	0
5	NAG	A	710	14/15	0.69	0.16	84,88,94,95	0
5	NAG	A	711	14/15	0.71	0.17	68,71,74,78	0
5	NAG	B	707	14/15	0.78	0.13	71,72,74,74	0
5	NAG	A	709	14/15	0.79	0.16	70,73,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	703	5/5	0.86	0.17	76,77,78,79	0
2	TRP	B	701	15/15	0.86	0.16	45,48,52,59	0
4	CA	B	704	1/1	0.89	0.10	102,102,102,102	0
3	PO4	B	703	5/5	0.90	0.14	72,72,74,75	0
3	PO4	B	702	5/5	0.92	0.09	59,60,60,65	0
4	CA	A	706	1/1	0.92	0.13	83,83,83,83	0
4	CA	B	705	1/1	0.93	0.14	81,81,81,81	0
2	TRP	A	701	15/15	0.94	0.09	18,28,30,57	0
4	CA	B	706	1/1	0.96	0.12	111,111,111,111	0
4	CA	A	705	1/1	0.96	0.13	56,56,56,56	0
3	PO4	A	702	5/5	0.97	0.07	26,30,33,35	0
4	CA	A	704	1/1	0.98	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.