



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3NCE / pdb_00003nce
Title : A mutant human Prolactin receptor antagonist H27A in complex with the mutant extracellular domain H188A of the human prolactin receptor
Authors : Kulkarni, M.V.; Tettamanzi, M.C.; Murphy, J.W.; Keeler, C.; Myszkka, D.G.; Chayen, N.E.; Lolis, E.J.; Hodsdon, M.E.
Deposited on : 2010-06-04
Resolution : 2.00 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

<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)
Validation Pipeline (wwPDB-VP)	:	2.49

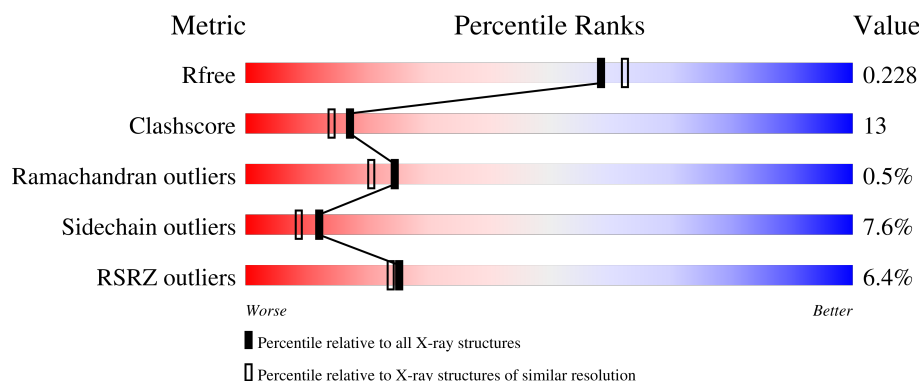
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	186	9% 69% 25% 5%
2	B	210	4% 75% 19% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3727 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 Prolactin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	10	0
			1561	983	270	298	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	initiating methionine	UNP P01236
A	27	ALA	HIS	engineered mutation	UNP P01236
A	129	ARG	GLY	engineered mutation	UNP P01236

- Molecule 2 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	4	0
			1700	1107	276	306	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P16471
B	188	ALA	HIS	engineered mutation	UNP P16471

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	4	Total	Na	0	0
			4	4		

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

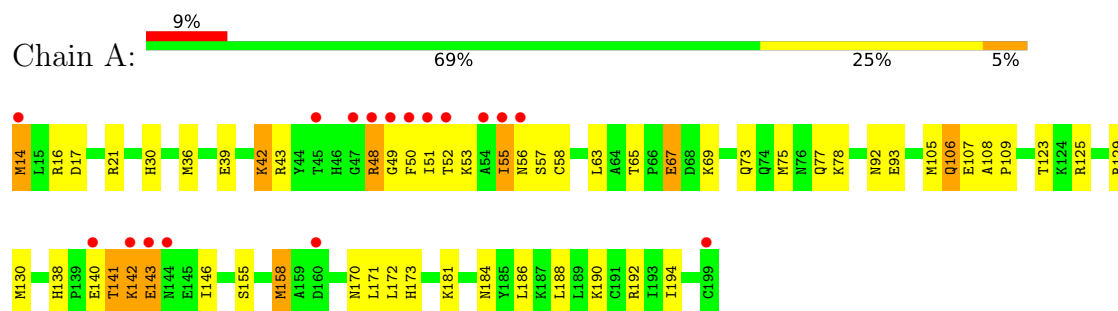
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	209	Total	O	0	0
			209	209		
6	B	243	Total	O	0	0
			243	243		

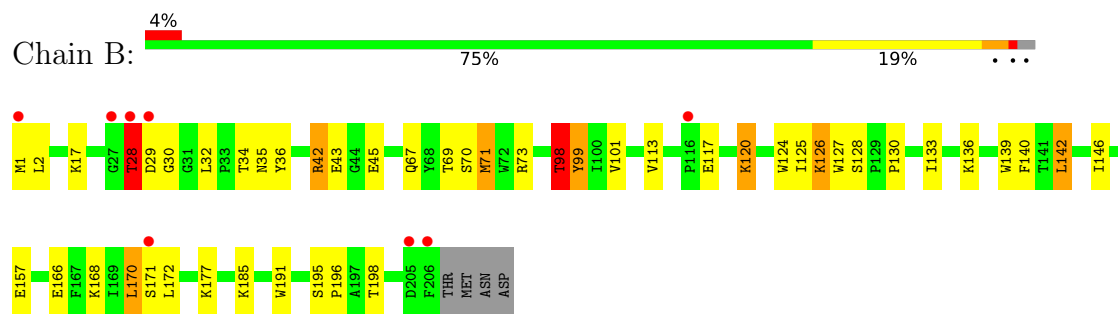
3 Residue-property plots [i](#)

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: Prolactin



- Molecule 2: Prolactin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	123.28Å 123.28Å 72.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.95 – 2.00 31.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.95-2.00) 99.9 (31.95-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.68 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.227 0.177 , 0.228	Depositor DCC
R_{free} test set	2160 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3727	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CO3, CL

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	1.45	6/1621 (0.4%)	1.35	15/2186 (0.7%)
2	B	1.58	9/1776 (0.5%)	1.31	10/2424 (0.4%)
All	All	1.52	15/3397 (0.4%)	1.33	25/4610 (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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	THR	CA-CB	10.82	1.70	1.53
2	B	98	THR	CB-OG1	9.93	1.59	1.43
2	B	69	THR	CA-C	6.09	1.59	1.52
2	B	98	THR	N-CA	-5.93	1.39	1.46
1	A	16	ARG	CD-NE	-5.69	1.38	1.46
2	B	128	SER	N-CA	5.68	1.50	1.45
1	A	93	GLU	C-O	5.66	1.30	1.24
1	A	55	ILE	CA-CB	5.53	1.60	1.54
2	B	101	VAL	CA-C	5.53	1.59	1.52
1	A	192	ARG	CD-NE	-5.52	1.38	1.46
1	A	188	LEU	CA-CB	5.46	1.61	1.53
2	B	28	THR	CA-C	5.34	1.59	1.52
2	B	125	ILE	N-CA	5.27	1.52	1.46
1	A	170	ASN	N-CA	-5.12	1.40	1.46
2	B	125	ILE	CA-CB	-5.02	1.48	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-11.93	108.46	119.20
1	A	16	ARG	NE-CZ-NH1	9.98	131.48	121.50
2	B	170	LEU	CA-C-N	-8.13	111.56	122.85
2	B	170	LEU	C-N-CA	-8.13	111.56	122.85
1	A	57	SER	N-CA-CB	-7.54	101.09	111.65
1	A	39	GLU	N-CA-C	7.41	119.36	111.28
1	A	192	ARG	CB-CG-CD	-7.30	94.52	111.30
1	A	16	ARG	CD-NE-CZ	7.06	134.29	124.40
1	A	192	ARG	NE-CZ-NH2	-7.02	112.88	119.20
2	B	98	THR	CB-CA-C	6.63	121.95	110.68
2	B	99	TYR	CA-CB-CG	-6.09	102.94	113.90
1	A	181	LYS	CB-CA-C	-6.06	100.73	110.79
1	A	16	ARG	CB-CG-CD	5.69	124.38	111.30
1	A	65	THR	CA-C-N	-5.48	114.28	119.76
1	A	65	THR	C-N-CA	-5.48	114.28	119.76
2	B	30	GLY	N-CA-C	-5.33	102.91	111.59
1	A	56	ASN	N-CA-C	5.26	122.01	110.80
1	A	106	GLN	CA-C-N	-5.15	115.29	123.12
1	A	106	GLN	C-N-CA	-5.15	115.29	123.12
2	B	28	THR	CB-CA-C	5.11	118.56	110.19
2	B	120	LYS	CA-C-N	-5.06	115.35	120.31
2	B	120	LYS	C-N-CA	-5.06	115.35	120.31
2	B	71	MET	CB-CG-SD	-5.05	97.53	112.70
2	B	98	THR	CA-CB-CG2	-5.02	101.97	110.50
1	A	173	HIS	N-CA-C	-5.01	105.89	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	THR	Peptide

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	1561	0	1564	33	0
2	B	1700	0	1642	52	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
4	A	8	0	0	0	0
5	B	1	0	0	0	0
6	A	209	0	0	9	1
6	B	243	0	0	14	1
All	All	3727	0	3206	82	1

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 13.

All (82) 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:155[A]:SER:OG	6:A:317:HOH:O	1.71	1.08
2:B:42[B]:ARG:NH1	2:B:42[B]:ARG:HG2	1.50	1.08
2:B:42[B]:ARG:HG2	2:B:42[B]:ARG:HH11	0.87	1.04
2:B:42[B]:ARG:HH11	2:B:42[B]:ARG:CG	1.70	1.02
1:A:105:MET:HE2	6:A:232:HOH:O	1.65	0.93
1:A:51:ILE:HD11	6:B:227:HOH:O	1.72	0.88
1:A:105:MET:CE	6:A:232:HOH:O	2.22	0.84
2:B:71:MET:CE	2:B:98:THR:HG23	2.11	0.80
2:B:45:GLU:HG3	2:B:73:ARG:HH11	1.48	0.78
2:B:171:SER:O	2:B:172:LEU:HD23	1.87	0.73
2:B:140:PHE:HE1	2:B:142:LEU:HD13	1.57	0.69
1:A:130:MET:SD	1:A:186[A]:LEU:HD21	2.33	0.68
2:B:130:PRO:HG2	2:B:133:ILE:HD12	1.76	0.68
1:A:92[A]:ASN:OD1	6:A:257:HOH:O	2.12	0.68
2:B:124:TRP:CZ3	2:B:168:LYS:HE3	2.29	0.68
1:A:14:MET:N	6:A:436:HOH:O	2.26	0.67
2:B:71:MET:HE3	2:B:98:THR:HG23	1.76	0.67
2:B:157:GLU:HG3	6:B:262:HOH:O	1.95	0.66
1:A:63:LEU:O	6:A:273:HOH:O	2.11	0.66
2:B:36:TYR:O	6:B:425:HOH:O	2.14	0.65
1:A:36:MET:HE3	1:A:172:LEU:HD22	1.79	0.65
2:B:45:GLU:HG3	2:B:73:ARG:NH1	2.13	0.63
1:A:48:ARG:NH1	1:A:49:GLY:H	1.98	0.62
1:A:14:MET:HB3	6:A:243:HOH:O	2.00	0.62
2:B:117:GLU:H	2:B:117:GLU:CD	2.07	0.61
1:A:67:GLU:HG2	2:B:70:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:GLU:CD	2:B:73:ARG:HH12	2.09	0.61
2:B:17:LYS:HD2	2:B:71:MET:HE2	1.82	0.61
2:B:42[B]:ARG:NH1	2:B:42[B]:ARG:CG	2.35	0.58
2:B:124:TRP:HZ3	2:B:168:LYS:HG3	1.67	0.58
2:B:124:TRP:CZ3	2:B:168:LYS:HG3	2.37	0.58
2:B:45:GLU:CG	2:B:73:ARG:NH1	2.67	0.57
1:A:58:CYS:HB3	6:A:213:HOH:O	2.05	0.57
2:B:198:THR:HG22	6:B:408:HOH:O	2.07	0.55
1:A:69:LYS:O	1:A:73:GLN:HG3	2.06	0.55
2:B:71:MET:HE1	2:B:98:THR:HG23	1.86	0.55
1:A:138:HIS:O	1:A:141:THR:HG23	2.06	0.55
2:B:140:PHE:CE1	2:B:142:LEU:HD13	2.40	0.54
2:B:45:GLU:CD	2:B:73:ARG:NH1	2.65	0.54
2:B:29:ASP:N	6:B:432:HOH:O	2.40	0.53
2:B:45:GLU:CG	2:B:73:ARG:HH11	2.20	0.53
2:B:34:THR:O	2:B:35[B]:ASN:ND2	2.42	0.53
1:A:49:GLY:O	1:A:53:LYS:HD2	2.09	0.52
1:A:48:ARG:HB2	1:A:50:PHE:CE2	2.45	0.52
2:B:126:LYS:NZ	6:B:436:HOH:O	2.43	0.51
2:B:124:TRP:CH2	2:B:166:GLU:CD	2.89	0.50
2:B:177:LYS:NZ	6:B:311:HOH:O	2.45	0.50
2:B:67[B]:GLN:NE2	6:B:248:HOH:O	2.45	0.49
1:A:190:LYS:HG3	1:A:194:ILE:HD12	1.94	0.49
1:A:48:ARG:HB2	1:A:50:PHE:HE2	1.78	0.48
1:A:21:ARG:HD2	1:A:21:ARG:O	2.15	0.47
1:A:143:GLU:O	1:A:143:GLU:HG2	2.15	0.47
2:B:177:LYS:HE2	6:B:311:HOH:O	2.14	0.47
2:B:195:SER:HB2	2:B:196:PRO:HD2	1.96	0.46
2:B:42[A]:ARG:HG3	2:B:42[A]:ARG:NH1	2.30	0.45
1:A:69:LYS:HB3	2:B:139:TRP:CD2	2.51	0.45
1:A:78:LYS:NZ	1:A:141:THR:HG22	2.31	0.45
1:A:171:LEU:C	1:A:171:LEU:HD23	2.42	0.45
2:B:28:THR:C	6:B:432:HOH:O	2.60	0.45
2:B:17:LYS:HD2	2:B:71:MET:CE	2.47	0.44
2:B:28:THR:HG23	2:B:29:ASP:OD1	2.17	0.44
2:B:124:TRP:CZ3	2:B:168:LYS:CG	3.00	0.44
2:B:124:TRP:CE3	2:B:168:LYS:HG2	2.52	0.44
2:B:198:THR:HG23	6:B:457:HOH:O	2.17	0.43
2:B:124:TRP:HH2	2:B:166:GLU:CD	2.26	0.43
1:A:77:GLN:HE21	1:A:138:HIS:CE1	2.37	0.43
2:B:71:MET:HE3	2:B:71:MET:HB3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42[A]:ARG:HG3	2:B:42[A]:ARG:HH11	1.85	0.42
1:A:14:MET:HE3	1:A:17:ASP:CG	2.43	0.42
1:A:55:ILE:HG21	6:B:271:HOH:O	2.19	0.42
1:A:158:MET:HB3	1:A:158:MET:HE3	1.71	0.42
1:A:123:THR:HG22	6:A:257:HOH:O	2.20	0.42
2:B:42[A]:ARG:HH11	2:B:42[A]:ARG:CG	2.33	0.41
2:B:127:TRP:CZ3	2:B:146:ILE:HD11	2.55	0.41
1:A:42:LYS:HE3	1:A:43:ARG:HB2	2.02	0.41
1:A:108:ALA:HA	1:A:109:PRO:HD2	1.90	0.41
2:B:136:LYS:HG3	6:B:288:HOH:O	2.21	0.41
2:B:185:LYS:HD2	2:B:191:TRP:CE2	2.56	0.41
1:A:30:HIS:HE1	2:B:99:TYR:OH	2.04	0.41
1:A:43:ARG:HG2	1:A:43:ARG:O	2.21	0.41
2:B:177:LYS:CE	6:B:311:HOH:O	2.69	0.41
2:B:42[B]:ARG:NH2	2:B:70:SER:OG	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:208:HOH:O	6:B:349:HOH:O[4_445]	2.04	0.16

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	194/186 (104%)	182 (94%)	10 (5%)	2 (1%)	12	8
2	B	208/210 (99%)	203 (98%)	5 (2%)	0	100	100
All	All	402/396 (102%)	385 (96%)	15 (4%)	2 (0%)	24	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	142	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/172 (106%)	167 (92%)	15 (8%)	10	7
2	B	187/189 (99%)	174 (93%)	13 (7%)	14	10
All	All	369/361 (102%)	341 (92%)	28 (8%)	12	9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	42	LYS
1	A	52	THR
1	A	67	GLU
1	A	75	MET
1	A	106	GLN
1	A	107	GLU
1	A	125	ARG
1	A	129	ARG
1	A	140	GLU
1	A	142	LYS
1	A	143	GLU
1	A	146	ILE
1	A	158	MET
1	A	184	ASN
2	B	1	MET
2	B	2	LEU
2	B	28	THR
2	B	32	LEU
2	B	42[A]	ARG
2	B	42[B]	ARG
2	B	43	GLU

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Mol	Chain	Res	Type
2	B	98	THR
2	B	113	VAL
2	B	120	LYS
2	B	126	LYS
2	B	142	LEU
2	B	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	138	HIS
1	A	173	HIS
2	B	115	GLN
2	B	164	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
4	CO3	A	7	-	3,3,3	0.83	0	2,3,3	0.60	0
4	CO3	A	6	-	3,3,3	1.31	0	2,3,3	1.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	186/186 (100%)	0.25	17 (9%) 15 13	11, 31, 73, 95	11 (5%)
2	B	206/210 (98%)	0.10	8 (3%) 43 42	19, 30, 54, 74	4 (1%)
All	All	392/396 (98%)	0.17	25 (6%) 25 24	11, 30, 66, 95	15 (3%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ILE	6.3
1	A	55	ILE	5.7
1	A	52	THR	5.1
1	A	54	ALA	4.6
2	B	28	THR	4.6
1	A	49	GLY	4.6
2	B	171	SER	3.9
1	A	48	ARG	3.6
1	A	142	LYS	3.6
1	A	50	PHE	3.4
2	B	1	MET	3.1
1	A	160	ASP	2.9
1	A	144	ASN	2.9
1	A	199	CYS	2.7
1	A	45	THR	2.4
1	A	56	ASN	2.4
2	B	116	PRO	2.3
2	B	206	PHE	2.3
2	B	29	ASP	2.2
1	A	143	GLU	2.2
1	A	14	MET	2.2
1	A	140	GLU	2.2
1	A	47	GLY	2.1
2	B	205	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	27	GLY	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
4	CO3	A	7	4/4	0.90	0.10	63,63,64,64	0
4	CO3	A	6	4/4	0.92	0.16	43,44,47,48	0
3	NA	B	215	1/1	0.93	0.07	55,55,55,55	0
3	NA	A	5	1/1	0.98	0.05	23,23,23,23	0
5	CL	B	213	1/1	0.98	0.04	30,30,30,30	0
3	NA	B	212	1/1	0.99	0.02	26,26,26,26	0
3	NA	B	214	1/1	0.99	0.04	33,33,33,33	0
3	NA	B	211	1/1	0.99	0.11	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.