



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:34 AM EDT

PDB ID : 2GL8 / pdb_00002gl8
Title : Human Retinoic acid receptor RXR-gamma ligand-binding domain
Authors : Min, J.R.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2006-04-04
Resolution : 2.40 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
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

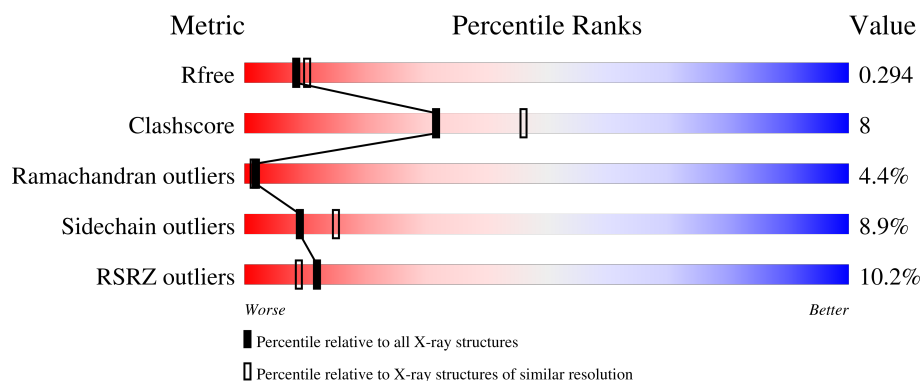
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	241	8% 54% 19% 6% 21%
1	B	241	5% 59% 19% • 20%
1	C	241	9% 63% 14% •• 20%
1	D	241	11% 65% 13% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5916 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 Retinoic acid receptor RXR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1459	931	254	268	6			
1	B	192	Total	C	N	O	S	0	0	0
			1454	928	257	263	6			
1	C	194	Total	C	N	O	S	0	0	0
			1447	919	256	266	6			
1	D	195	Total	C	N	O	S	0	0	0
			1451	920	254	271	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P48443
A	2	SER	-	cloning artifact	UNP P48443
A	3	HIS	-	cloning artifact	UNP P48443
A	4	ASN	-	cloning artifact	UNP P48443
B	1	GLY	-	cloning artifact	UNP P48443
B	2	SER	-	cloning artifact	UNP P48443
B	3	HIS	-	cloning artifact	UNP P48443
B	4	ASN	-	cloning artifact	UNP P48443
C	1	GLY	-	cloning artifact	UNP P48443
C	2	SER	-	cloning artifact	UNP P48443
C	3	HIS	-	cloning artifact	UNP P48443
C	4	ASN	-	cloning artifact	UNP P48443
D	1	GLY	-	cloning artifact	UNP P48443
D	2	SER	-	cloning artifact	UNP P48443
D	3	HIS	-	cloning artifact	UNP P48443
D	4	ASN	-	cloning artifact	UNP P48443

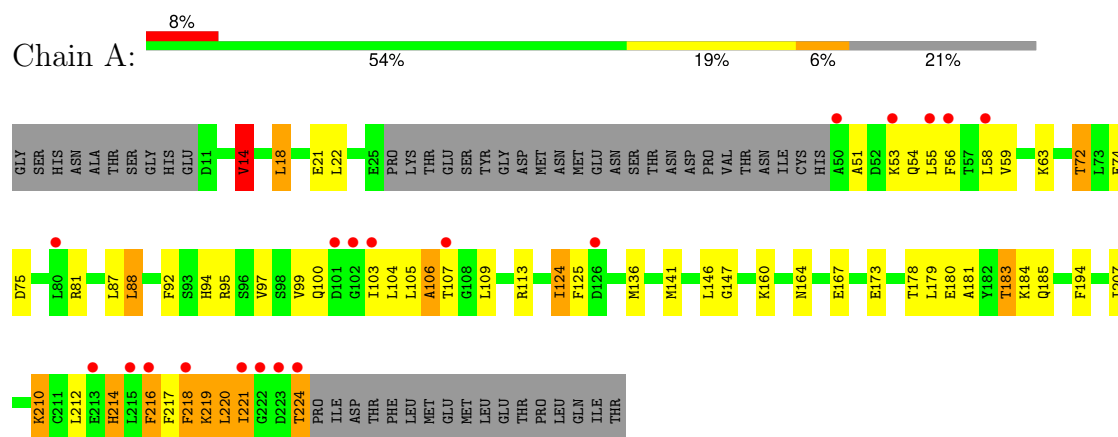
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	B	23	Total 23	O 23	0	0
2	C	27	Total 27	O 27	0	0
2	D	23	Total 23	O 23	0	0

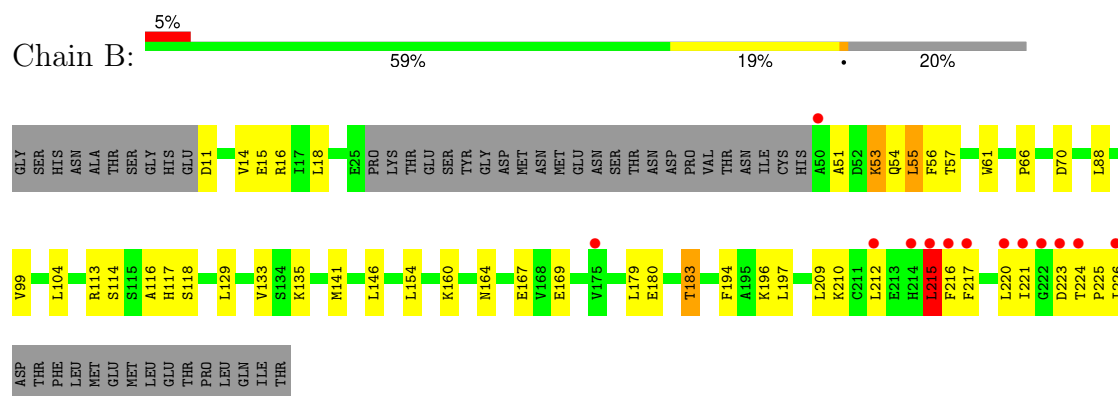
3 Residue-property plots [i](#)

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.

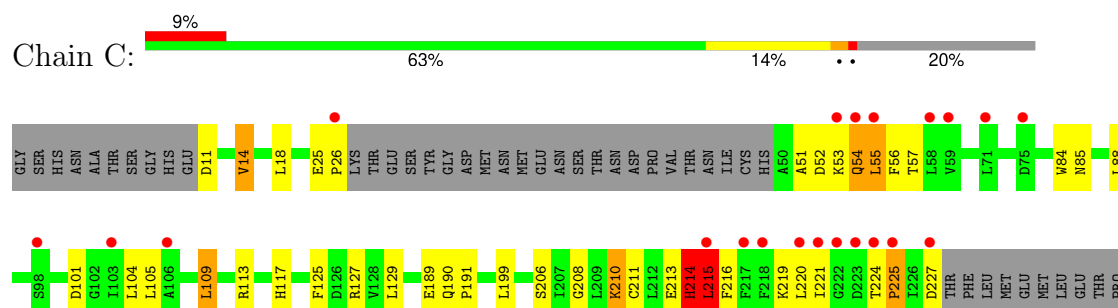
• Molecule 1: Retinoic acid receptor RXR-gamma



• Molecule 1: Retinoic acid receptor RXR-gamma

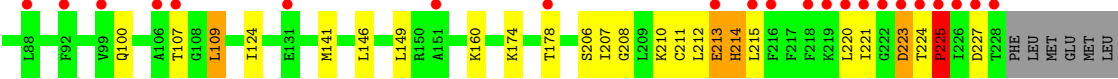


• Molecule 1: Retinoic acid receptor RXR-gamma



LEU
GLN
ILE
THR

● Molecule 1: Retinoic acid receptor RXR-gamma



GLU
THR
PRO
LEU
GLN
ILE
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.07Å 161.32Å 68.68Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 80.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (80.58-2.40) 99.0 (80.58-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.296 0.242 , 0.294	Depositor DCC
R_{free} test set	1936 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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

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	0.84	2/1484 (0.1%)	1.12	6/2005 (0.3%)
1	B	0.91	3/1480 (0.2%)	1.03	3/2001 (0.1%)
1	C	0.73	1/1473 (0.1%)	1.04	4/1989 (0.2%)
1	D	0.65	0/1475	1.05	3/1996 (0.2%)
All	All	0.79	6/5912 (0.1%)	1.06	16/7991 (0.2%)

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	2
1	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	ILE	C-O	17.39	1.58	1.23
1	C	26	PRO	C-O	9.17	1.41	1.23
1	A	224	THR	C-O	8.91	1.41	1.23
1	B	212	LEU	C-O	8.32	1.33	1.24
1	B	212	LEU	CG-CD2	5.65	1.71	1.52
1	A	224	THR	CB-CG2	5.39	1.70	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	PRO	N-CA-CB	9.59	113.15	102.60
1	A	224	THR	CA-C-O	-6.57	109.63	120.80
1	A	99	VAL	N-CA-C	5.73	117.45	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	PHE	N-CA-C	5.65	117.65	109.07
1	D	223	ASP	N-CA-C	5.65	117.64	108.26
1	C	224	THR	CA-C-N	5.63	126.88	119.84
1	C	224	THR	C-N-CA	5.63	126.88	119.84
1	B	55	LEU	N-CA-C	-5.63	98.81	110.80
1	A	14	VAL	CB-CA-C	-5.61	104.56	112.14
1	C	214	HIS	N-CA-C	5.42	122.35	110.80
1	C	14	VAL	CB-CA-C	-5.36	103.86	112.16
1	D	213	GLU	N-CA-C	-5.25	106.64	112.57
1	A	221	ILE	N-CA-C	5.23	120.21	109.34
1	A	219	LYS	CA-C-N	5.16	130.99	121.70
1	A	219	LYS	C-N-CA	5.16	130.99	121.70
1	B	226	ILE	CA-C-O	-5.02	112.27	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	HIS	Peptide
1	B	53	LYS	Peptide
1	B	54	GLN	Peptide
1	D	223	ASP	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	1459	0	1470	39	0
1	B	1454	0	1454	20	0
1	C	1447	0	1434	18	0
1	D	1451	0	1424	20	0
2	A	32	0	0	0	0
2	B	23	0	0	0	0
2	C	27	0	0	0	0
2	D	23	0	0	0	0
All	All	5916	0	5782	94	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 8.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HG	1:B:216:PHE:H	1.35	0.89
1:A:94:HIS:HD2	1:A:141:MET:HE2	1.40	0.86
1:A:219:LYS:HA	1:A:220:LEU:HB2	1.57	0.84
1:A:219:LYS:HA	1:A:220:LEU:CB	2.16	0.76
1:A:72:THR:HG22	1:A:75:ASP:H	1.51	0.76
1:A:219:LYS:CA	1:A:220:LEU:HB2	2.16	0.75
1:A:164:ASN:ND2	1:A:167:GLU:HG3	2.04	0.73
1:B:215:LEU:HG	1:B:216:PHE:N	2.07	0.68
1:A:124:ILE:HD11	1:A:207:ILE:HG23	1.74	0.68
1:C:206:SER:O	1:C:210:LYS:HD2	1.93	0.68
1:B:183:THR:HG21	1:B:194:PHE:HB2	1.74	0.68
1:A:164:ASN:HD22	1:A:167:GLU:HG3	1.60	0.66
1:A:181:ALA:O	1:A:185:GLN:HG3	1.95	0.65
1:D:141:MET:HE2	1:D:146:LEU:HA	1.79	0.65
1:A:94:HIS:CD2	1:A:141:MET:HE2	2.30	0.63
1:C:53:LYS:HA	1:C:55:LEU:H	1.62	0.63
1:C:189:GLU:HG2	1:C:190:GLN:HG3	1.81	0.63
1:A:14:VAL:HG22	1:A:178:THR:HG23	1.80	0.61
1:A:103:ILE:HD12	1:A:125:PHE:CE2	2.35	0.61
1:A:141:MET:HE3	1:A:146:LEU:HB2	1.82	0.60
1:A:217:PHE:O	1:A:218:PHE:HB2	2.01	0.60
1:D:224:THR:CA	1:D:225:PRO:CB	2.79	0.60
1:D:124:ILE:HD11	1:D:207:ILE:HG23	1.84	0.60
1:D:72:THR:HG22	1:D:75:ASP:H	1.68	0.58
1:D:141:MET:CE	1:D:149:LEU:HD12	2.32	0.58
1:A:136:MET:HE2	1:A:141:MET:HE1	1.87	0.57
1:A:210:LYS:HE3	1:B:209:LEU:HD13	1.86	0.56
1:D:141:MET:HE2	1:D:146:LEU:CA	2.35	0.56
1:A:173:GLU:OE1	1:B:196:LYS:NZ	2.37	0.56
1:B:180:GLU:O	1:B:183:THR:HG22	2.06	0.54
1:A:54:GLN:C	1:A:56:PHE:H	2.15	0.54
1:D:84:TRP:CD1	1:D:85:ASN:N	2.76	0.54
1:D:25:GLU:N	1:D:26:PRO:HA	2.23	0.53
1:D:141:MET:HE1	1:D:149:LEU:HD12	1.91	0.52
1:B:223:ASP:O	1:B:225:PRO:HD3	2.12	0.50
1:A:141:MET:HE1	1:A:146:LEU:HD13	1.93	0.50
1:B:113:ARG:HG2	1:B:117:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLN:C	1:C:56:PHE:H	2.21	0.49
1:A:219:LYS:CB	1:A:220:LEU:HB2	2.43	0.49
1:C:105:LEU:HB2	1:C:109:LEU:HB2	1.94	0.49
1:B:225:PRO:HG2	1:D:59:VAL:HG21	1.95	0.48
1:A:18:LEU:HD22	1:A:22:LEU:HG	1.96	0.48
1:D:81:ARG:HA	1:D:84:TRP:HE3	1.79	0.47
1:A:94:HIS:CD2	1:A:141:MET:CE	2.95	0.47
1:A:179:LEU:O	1:A:183:THR:HB	2.15	0.47
1:A:55:LEU:HD22	1:A:88:LEU:HD11	1.96	0.46
1:C:125:PHE:CE1	1:C:129:LEU:HD11	2.49	0.46
1:D:141:MET:HE3	1:D:149:LEU:HD12	1.98	0.46
1:D:211:CYS:C	1:D:213:GLU:H	2.23	0.46
1:C:189:GLU:O	1:C:191:PRO:HD3	2.15	0.46
1:A:180:GLU:O	1:A:184:LYS:HG3	2.16	0.46
1:B:16:ARG:HD3	1:B:66:PRO:HG3	1.98	0.46
1:B:164:ASN:ND2	1:B:167:GLU:CB	2.79	0.46
1:A:183:THR:HG21	1:A:194:PHE:HB2	1.97	0.46
1:B:113:ARG:HG2	1:B:117:HIS:CD2	2.50	0.46
1:C:113:ARG:HG2	1:C:117:HIS:HD2	1.81	0.45
1:A:21:GLU:OE2	1:A:147:GLY:HA2	2.16	0.45
1:D:85:ASN:ND2	1:D:208:GLY:O	2.49	0.45
1:B:164:ASN:HD22	1:B:167:GLU:CB	2.29	0.45
1:C:225:PRO:C	1:C:227:ASP:H	2.24	0.45
1:A:58:LEU:HD11	1:A:87:LEU:HD13	1.98	0.45
1:A:219:LYS:HA	1:A:220:LEU:CG	2.45	0.45
1:A:92:PHE:CD1	1:A:92:PHE:C	2.94	0.45
1:C:85:ASN:HD21	1:C:211:CYS:HB2	1.82	0.45
1:B:61:TRP:CZ3	1:B:154:LEU:HD22	2.52	0.45
1:C:213:GLU:C	1:C:214:HIS:HD1	2.26	0.44
1:A:105:LEU:O	1:A:107:THR:N	2.50	0.44
1:A:124:ILE:HD13	1:A:210:LYS:HB3	2.00	0.43
1:A:210:LYS:HE2	1:A:210:LYS:N	2.33	0.43
1:C:215:LEU:HD13	1:C:216:PHE:H	1.83	0.43
1:B:179:LEU:HD11	1:B:197:LEU:HD13	1.99	0.43
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.79	0.43
1:A:59:VAL:HG12	1:A:63:LYS:HD2	2.00	0.43
1:A:72:THR:HG23	1:A:74:GLU:OE2	2.18	0.43
1:A:95:ARG:CZ	1:A:106:ALA:HB2	2.49	0.43
1:B:129:LEU:HA	1:B:133:VAL:HB	2.01	0.43
1:C:127:ARG:NH1	1:C:210:LYS:HD3	2.34	0.42
1:A:141:MET:CE	1:A:146:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:ND2	1:C:208:GLY:O	2.53	0.42
1:C:214:HIS:O	1:C:215:LEU:O	2.38	0.42
1:D:80:LEU:O	1:D:84:TRP:HB3	2.18	0.42
1:C:213:GLU:C	1:C:214:HIS:ND1	2.77	0.42
1:D:213:GLU:O	1:D:214:HIS:HB2	2.20	0.41
1:C:215:LEU:HD13	1:C:216:PHE:N	2.35	0.41
1:B:141:MET:HE3	1:B:146:LEU:HB2	2.02	0.41
1:D:12:MET:O	1:D:178:THR:HG21	2.20	0.41
1:B:141:MET:HE3	1:B:146:LEU:HA	2.02	0.41
1:B:116:ALA:C	1:B:118:SER:N	2.79	0.41
1:A:105:LEU:C	1:A:107:THR:H	2.29	0.41
1:B:116:ALA:C	1:B:118:SER:H	2.27	0.41
1:D:24:VAL:C	1:D:26:PRO:HA	2.46	0.41
1:D:84:TRP:CD1	1:D:84:TRP:C	2.98	0.40
1:A:212:LEU:C	1:A:214:HIS:H	2.29	0.40
1:D:107:THR:OG1	1:D:109:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	186/241 (77%)	169 (91%)	9 (5%)	8 (4%)	2	1
1	B	188/241 (78%)	168 (89%)	13 (7%)	7 (4%)	2	2
1	C	190/241 (79%)	170 (90%)	8 (4%)	12 (6%)	1	0
1	D	191/241 (79%)	178 (93%)	7 (4%)	6 (3%)	3	3
All	All	755/964 (78%)	685 (91%)	37 (5%)	33 (4%)	2	1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	218	PHE
1	A	220	LEU
1	B	51	ALA
1	B	53	LYS
1	B	221	ILE
1	C	52	ASP
1	C	54	GLN
1	C	215	LEU
1	D	225	PRO
1	D	227	ASP
1	A	51	ALA
1	A	53	LYS
1	A	106	ALA
1	B	55	LEU
1	B	215	LEU
1	B	220	LEU
1	C	51	ALA
1	C	55	LEU
1	C	219	LYS
1	D	220	LEU
1	D	221	ILE
1	C	101	ASP
1	C	109	LEU
1	C	220	LEU
1	C	225	PRO
1	D	212	LEU
1	D	214	HIS
1	C	214	HIS
1	C	221	ILE
1	A	216	PHE
1	B	99	VAL
1	A	221	ILE

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	155/211 (74%)	140 (90%)	15 (10%)	8	12
1	B	151/211 (72%)	134 (89%)	17 (11%)	5	8
1	C	150/211 (71%)	139 (93%)	11 (7%)	13	22
1	D	149/211 (71%)	138 (93%)	11 (7%)	13	22
All	All	605/844 (72%)	551 (91%)	54 (9%)	9	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	18	LEU
1	A	72	THR
1	A	81	ARG
1	A	88	LEU
1	A	97	VAL
1	A	104	LEU
1	A	109	LEU
1	A	113	ARG
1	A	124	ILE
1	A	160	LYS
1	A	183	THR
1	A	210	LYS
1	A	216	PHE
1	A	224	THR
1	B	11	ASP
1	B	14	VAL
1	B	15	GLU
1	B	18	LEU
1	B	56	PHE
1	B	57	THR
1	B	70	ASP
1	B	88	LEU
1	B	104	LEU
1	B	114	SER
1	B	135	LYS
1	B	160	LYS
1	B	169	GLU
1	B	183	THR
1	B	210	LYS
1	B	215	LEU
1	B	224	THR
1	C	11	ASP

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Mol	Chain	Res	Type
1	C	14	VAL
1	C	18	LEU
1	C	25	GLU
1	C	57	THR
1	C	84	TRP
1	C	88	LEU
1	C	104	LEU
1	C	210	LYS
1	C	214	HIS
1	C	215	LEU
1	D	14	VAL
1	D	18	LEU
1	D	72	THR
1	D	84	TRP
1	D	100	GLN
1	D	109	LEU
1	D	160	LYS
1	D	174	LYS
1	D	206	SER
1	D	210	LYS
1	D	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	110	HIS
1	A	185	GLN
1	B	100	GLN
1	B	117	HIS
1	B	164	ASN
1	C	76	GLN
1	C	85	ASN
1	C	117	HIS
1	C	156	ASN
1	D	112	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	190/241 (78%)	0.52	19 (10%) 12 9	41, 54, 74, 86	0
1	B	192/241 (79%)	0.51	13 (6%) 23 20	44, 63, 84, 87	0
1	C	194/241 (80%)	0.68	21 (10%) 11 8	43, 62, 75, 78	0
1	D	195/241 (80%)	0.78	26 (13%) 7 5	45, 69, 90, 95	0
All	All	771/964 (79%)	0.62	79 (10%) 12 9	41, 62, 85, 95	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	ALA	6.6
1	C	55	LEU	5.7
1	A	224	THR	5.5
1	B	226	ILE	4.7
1	B	216	PHE	4.5
1	B	215	LEU	4.3
1	A	215	LEU	4.2
1	C	224	THR	4.1
1	C	220	LEU	3.9
1	D	226	ILE	3.8
1	B	223	ASP	3.7
1	B	217	PHE	3.7
1	B	221	ILE	3.6
1	C	225	PRO	3.6
1	C	75	ASP	3.6
1	D	216	PHE	3.5
1	D	218	PHE	3.5
1	D	220	LEU	3.5
1	A	221	ILE	3.5
1	C	218	PHE	3.4
1	A	107	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	3.3
1	C	227	ASP	3.2
1	A	216	PHE	3.2
1	A	55	LEU	3.2
1	B	214	HIS	3.2
1	D	225	PRO	3.1
1	D	221	ILE	3.1
1	A	101	ASP	3.0
1	C	223	ASP	3.0
1	C	215	LEU	2.9
1	C	54	GLN	2.9
1	A	126	ASP	2.8
1	B	220	LEU	2.7
1	A	103	ILE	2.7
1	C	53	LYS	2.7
1	D	88	LEU	2.6
1	D	99	VAL	2.6
1	A	222	GLY	2.6
1	C	106	ALA	2.5
1	A	213	GLU	2.5
1	A	102	GLY	2.5
1	B	222	GLY	2.5
1	C	58	LEU	2.5
1	D	131	GLU	2.5
1	D	92	PHE	2.5
1	D	213	GLU	2.4
1	A	58	LEU	2.4
1	B	224	THR	2.4
1	D	107	THR	2.4
1	C	103	ILE	2.4
1	C	59	VAL	2.4
1	D	222	GLY	2.3
1	D	178	THR	2.3
1	C	217	PHE	2.3
1	B	212	LEU	2.2
1	D	227	ASP	2.2
1	A	56	PHE	2.2
1	D	52	ASP	2.2
1	D	151	ALA	2.2
1	D	54	GLN	2.2
1	D	228	THR	2.2
1	C	71	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	224	THR	2.1
1	C	221	ILE	2.1
1	D	81	ARG	2.1
1	C	26	PRO	2.1
1	B	175	VAL	2.1
1	A	50	ALA	2.1
1	C	222	GLY	2.1
1	A	223	ASP	2.1
1	D	223	ASP	2.1
1	D	219	LYS	2.1
1	D	215	LEU	2.1
1	C	98	SER	2.0
1	A	218	PHE	2.0
1	A	80	LEU	2.0
1	D	51	ALA	2.0
1	A	53	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.