



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3OE8
Title : Crystal structure of the CXCR4 chemokine receptor in complex with a small molecule antagonist IT1t in P1 spacegroup
Authors : Wu, B.; Mol, C.D.; Han, G.W.; Katritch, V.; Chien, E.Y.T.; Liu, W.; Cherezov, V.; Stevens, R.C.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D); GPCR Network (GPCR)
Deposited on : 2010-08-12
Resolution : 3.10 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

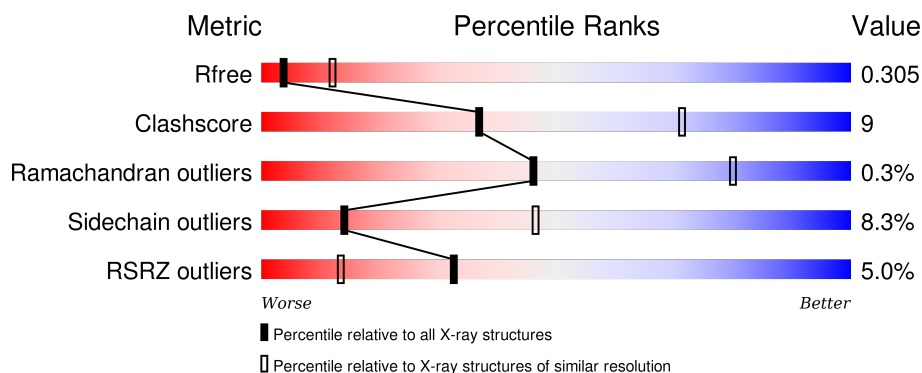
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	502	<div> <div>3%</div> <div>66%</div> <div>15%</div> <div>• •</div> <div>14%</div> </div>
1	B	502	<div> <div>6%</div> <div>68%</div> <div>14%</div> <div>•</div> <div>15%</div> </div>
1	C	502	<div> <div>4%</div> <div>72%</div> <div>12%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10373 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 C-X-C chemokine receptor type 4, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3459	2269	577	597	16			
1	B	426	Total	C	N	O	S	0	0	0
			3404	2240	570	578	16			
1	C	428	Total	C	N	O	S	0	0	0
			3429	2263	567	583	16			

There are 54 discrepancies between the modelled and reference sequences:

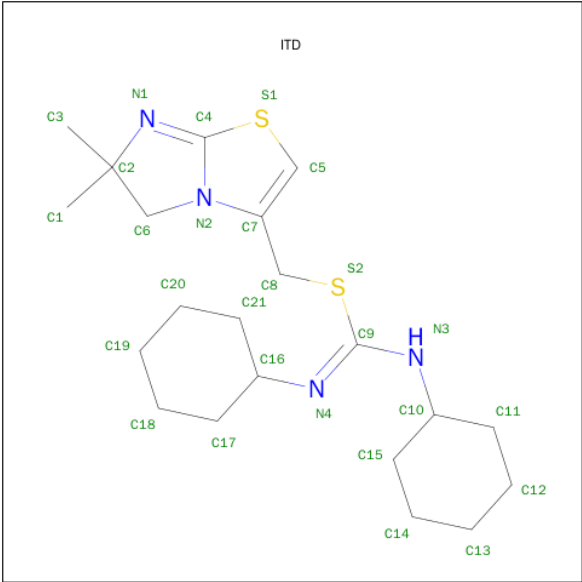
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
A	-2	ALA	-	expression tag	UNP P61073
A	-1	GLY	-	expression tag	UNP P61073
A	0	ALA	-	expression tag	UNP P61073
A	1	PRO	-	expression tag	UNP P61073
A	125	TRP	LEU	engineered	UNP P61073
A	900	GLY	-	linker	UNP P61073
A	901	SER	-	linker	UNP P61073
A	1200	GLY	-	linker	UNP P61073
A	1201	SER	-	linker	UNP P61073
A	1054	THR	CYS	engineered	UNP P00720
A	1097	ALA	CYS	engineered	UNP P00720
A	320	GLY	-	expression tag	UNP P61073
A	321	ARG	-	expression tag	UNP P61073
A	322	PRO	-	expression tag	UNP P61073
A	323	LEU	-	expression tag	UNP P61073
A	324	GLU	-	expression tag	UNP P61073

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	VAL	-	expression tag	UNP P61073
A	326	LEU	-	expression tag	UNP P61073
A	327	PHE	-	expression tag	UNP P61073
A	328	GLN	-	expression tag	UNP P61073
B	-9	ASP	-	expression tag	UNP P61073
B	-8	TYR	-	expression tag	UNP P61073
B	-7	LYS	-	expression tag	UNP P61073
B	-6	ASP	-	expression tag	UNP P61073
B	-5	ASP	-	expression tag	UNP P61073
B	-4	ASP	-	expression tag	UNP P61073
B	-3	ASP	-	expression tag	UNP P61073
B	-2	ALA	-	expression tag	UNP P61073
B	-1	GLY	-	expression tag	UNP P61073
B	0	ALA	-	expression tag	UNP P61073
B	1	PRO	-	expression tag	UNP P61073
B	125	TRP	LEU	engineered	UNP P61073
B	900	GLY	-	linker	UNP P61073
B	901	SER	-	linker	UNP P61073
B	1200	GLY	-	linker	UNP P61073
B	1201	SER	-	linker	UNP P61073
B	1054	THR	CYS	engineered	UNP P00720
B	1097	ALA	CYS	engineered	UNP P00720
B	320	GLY	-	expression tag	UNP P61073
B	321	ARG	-	expression tag	UNP P61073
B	322	PRO	-	expression tag	UNP P61073
B	323	LEU	-	expression tag	UNP P61073
B	324	GLU	-	expression tag	UNP P61073
B	325	VAL	-	expression tag	UNP P61073
B	326	LEU	-	expression tag	UNP P61073
B	327	PHE	-	expression tag	UNP P61073
B	328	GLN	-	expression tag	UNP P61073

- Molecule 2 is (6,6-DIMETHYL-5,6-DIHYDROIMIDAZO[2,1-B][1,3]THIAZOL-3-YL)METHYL N,N'-DICYCLOHEXYLIMIDOTHIOCARBAMATE (three-letter code: ITD) (formula: C₂₁H₃₄N₄S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			27	21	4	2		
2	B	1	Total	C	N	S	0	0
			27	21	4	2		
2	C	1	Total	C	N	S	0	0
			27	21	4	2		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:

66% 15% 3% 14%

ASP TYR LYS ASP ASP ASP GLY ALA PRO GLU ILE SER TYR THR SER ASP ASN TYR THR GLU GLU MET GLY SER GLY ASP TYR ASP SER MET LYS GLU P27 C28 PHE ARG GLU GLU ASN ALA P35 P39 I53 I60 L61 V62 H63 G64 V65 D66 R67 V68 D69

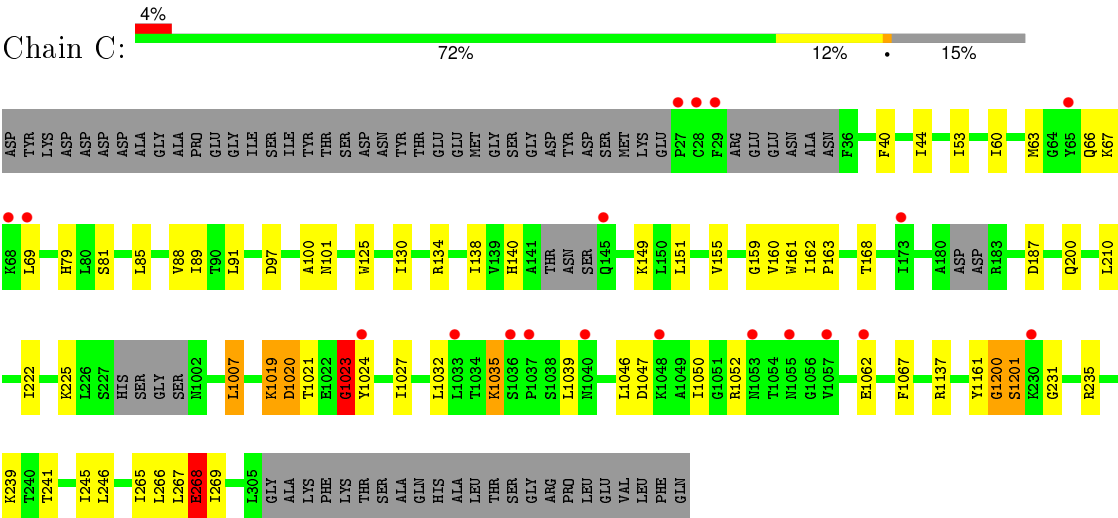
R70 K75 L85 D97 A98 V99 M100 M101 Y102 Y103 C109 V114 L132 D133 R134 A137 I138 V139 H140 A141 T142 M143 S144 Q145 R146 P147 R148 V156 Y157 V158 P163 A164 L165 L166 L167 T168 D171 F172 I173 F174 E179 L181 D181 D182 Y184 I185 C186 D187

R188 Y190 W195 I215 Y219 I223 K224 K225 H228 S229 G290 S901 M1002 I1003 F1004 S1005 M1006 L1007 R1008 LYS K1016 V1057 E1064 G1077 K1083 V1094 T1115 R1125 E1128 M1132 R1137 I1140 Q1141 W1158 Y1161 GLY SER LYS GLY H232

I245 D262 S263 F264 I265 L266 E268 I269 Q272 G273 C274 E275 F276 E277 V280 Y302 L305 GLY LYS PHE LYS THR SER ALA GLN HIS ALA LEU THR SER GLY ARG LEU LEU VAL LEU PHE GLN

- [illegible]

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.37Å 76.60Å 91.72Å 96.00° 97.78° 97.38°	Depositor
Resolution (Å)	19.97 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.97-3.10) 83.8 (19.97-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.09Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.250 , 0.295 0.251 , 0.305	Depositor DCC
R_{free} test set	1441 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28647 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10373	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: ITD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/3543	0.92	30/4814 (0.6%)
1	B	0.48	0/3485	0.77	12/4731 (0.3%)
1	C	0.50	3/3511 (0.1%)	0.85	16/4767 (0.3%)
All	All	0.49	3/10539 (0.0%)	0.85	58/14312 (0.4%)

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	C	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1201	SER	C-O	10.02	1.42	1.23
1	C	1201	SER	CA-C	-8.01	1.32	1.52
1	C	1200	GLY	CA-C	-6.40	1.41	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1201	SER	N-CA-C	13.97	148.71	111.00
1	C	1201	SER	CB-CA-C	-13.45	84.54	110.10
1	C	1201	SER	N-CA-C	13.16	146.55	111.00
1	A	232	HIS	N-CA-CB	-12.66	87.82	110.60
1	A	229	SER	O-C-N	-12.10	102.64	123.20
1	C	1201	SER	O-C-N	-12.08	103.37	122.70
1	C	101	ASN	N-CA-CB	-11.54	89.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	900	GLY	N-CA-C	11.42	141.65	113.10
1	A	232	HIS	N-CA-C	11.11	140.99	111.00
1	C	1023	GLY	N-CA-C	10.94	140.45	113.10
1	C	1200	GLY	C-N-CA	10.12	146.99	121.70
1	C	1201	SER	C-N-CA	10.11	146.97	121.70
1	C	100	ALA	CB-CA-C	-9.82	95.37	110.10
1	A	1005	GLU	CB-CA-C	-9.80	90.81	110.40
1	A	100	ALA	CB-CA-C	-9.79	95.42	110.10
1	A	229	SER	CA-C-N	9.68	135.55	116.20
1	A	173	ILE	CB-CA-C	-9.48	92.65	111.60
1	A	137	ALA	CB-CA-C	9.08	123.72	110.10
1	B	1201	SER	CB-CA-C	-8.99	93.02	110.10
1	C	269	ILE	N-CA-C	8.52	133.99	111.00
1	A	140	HIS	N-CA-CB	-8.40	95.48	110.60
1	C	268	GLU	N-CA-C	8.29	133.37	111.00
1	A	99	VAL	CB-CA-C	-8.26	95.70	111.40
1	B	257	ILE	CB-CA-C	-8.19	95.22	111.60
1	B	231	GLY	N-CA-C	-7.91	93.33	113.10
1	B	260	SER	CB-CA-C	-7.82	95.25	110.10
1	A	1006	MET	N-CA-C	-7.69	90.23	111.00
1	B	261	ILE	CB-CA-C	-7.53	96.55	111.60
1	A	101	ASN	N-CA-CB	-7.41	97.26	110.60
1	A	266	LEU	CB-CA-C	-7.26	96.41	110.20
1	A	139	VAL	CB-CA-C	7.24	125.16	111.40
1	A	183	ARG	N-CA-CB	7.23	123.61	110.60
1	C	1201	SER	CA-C-O	-7.10	105.19	120.10
1	B	208	LEU	N-CA-C	7.03	129.97	111.00
1	A	182	ASP	CB-CA-C	-6.76	96.87	110.40
1	A	141	ALA	CB-CA-C	-6.72	100.02	110.10
1	A	229	SER	C-N-CA	6.58	136.12	122.30
1	A	1115	THR	N-CA-C	6.40	128.28	111.00
1	A	173	ILE	N-CA-C	6.24	127.84	111.00
1	B	259	ILE	CB-CA-C	-6.23	99.15	111.60
1	A	100	ALA	N-CA-C	-6.22	94.20	111.00
1	C	100	ALA	N-CA-C	-6.09	94.55	111.00
1	A	144	SER	N-CA-CB	-5.88	101.68	110.50
1	C	1200	GLY	N-CA-C	5.82	127.65	113.10
1	B	1161	TYR	O-C-N	-5.82	113.31	123.20
1	C	67	LYS	CB-CA-C	5.78	121.95	110.40
1	B	208	LEU	N-CA-CB	-5.70	99.00	110.40
1	A	103	TYR	N-CA-CB	5.60	120.68	110.60
1	A	101	ASN	N-CA-C	5.54	125.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ILE	N-CA-CB	-5.53	98.08	110.80
1	A	141	ALA	N-CA-C	5.53	125.92	111.00
1	A	267	LEU	N-CA-C	-5.34	96.59	111.00
1	B	260	SER	N-CA-C	5.34	125.42	111.00
1	A	99	VAL	N-CA-C	5.29	125.28	111.00
1	B	74	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	C	1019	LYS	N-CA-C	-5.12	97.19	111.00
1	A	138	ILE	N-CA-CB	-5.10	99.08	110.80
1	A	268	GLU	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1200	GLY	Mainchain,Peptide
1	C	1201	SER	Mainchain

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	3459	0	3494	105	0
1	B	3404	0	3454	66	0
1	C	3429	0	3495	27	0
2	A	27	0	34	2	0
2	B	27	0	34	4	0
2	C	27	0	34	4	0
All	All	10373	0	10545	196	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 9.

All (196) 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:265:ILE:HG22	1:A:266:LEU:N	1.55	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:TYR:HE2	1:C:1035:LYS:HB3	1.19	1.06
1:A:143:ASN:ND2	1:A:143:ASN:H	1.52	1.06
1:C:267:LEU:O	1:C:268:GLU:HG3	1.59	1.01
1:C:1024:TYR:CE2	1:C:1035:LYS:HB3	1.96	1.01
1:C:66:GLN:O	1:C:66:GLN:HG2	1.60	1.00
1:A:146:ARG:N	1:A:147:PRO:HD2	1.72	1.00
1:B:261:ILE:HG22	1:B:262:ASP:N	1.77	0.99
1:A:137:ALA:HB2	1:A:148:ARG:CZ	1.92	0.98
1:B:208:LEU:HD22	1:B:256:TYR:CZ	2.01	0.94
1:A:1002:ASN:O	1:A:1158:TRP:CZ3	2.21	0.93
1:A:140:HIS:O	1:A:144:SER:HB3	1.68	0.93
1:A:265:ILE:CG2	1:A:266:LEU:N	2.31	0.93
1:B:259:ILE:HG22	1:B:260:SER:N	1.81	0.93
1:A:1004:PHE:CZ	1:A:1064:GLU:HG3	2.04	0.93
1:A:143:ASN:N	1:A:143:ASN:HD22	1.62	0.92
1:A:173:ILE:HG22	1:A:174:PHE:N	1.80	0.92
1:A:265:ILE:O	1:A:268:GLU:HA	1.73	0.89
1:B:1050:ILE:HD12	1:B:1062:GLU:HG2	1.56	0.88
1:A:1006:MET:HE2	1:A:1161:TYR:CZ	2.09	0.87
1:B:259:ILE:O	1:B:263:SER:CB	2.23	0.87
1:C:267:LEU:C	1:C:268:GLU:HG3	1.94	0.87
1:B:262:ASP:HB2	1:B:280:VAL:HG11	1.56	0.86
1:A:174:PHE:O	1:A:188:ARG:HA	1.74	0.86
1:B:60:ILE:HD12	1:B:85:LEU:HD22	1.56	0.86
1:C:66:GLN:CG	1:C:66:GLN:O	2.24	0.85
1:A:146:ARG:H	1:A:147:PRO:HD2	1.42	0.84
1:B:265:ILE:O	1:B:266:LEU:HG	1.77	0.82
1:A:181:ASP:O	1:A:182:ASP:CB	2.30	0.80
1:B:232:HIS:CD2	1:B:232:HIS:H	1.95	0.80
1:B:265:ILE:O	1:B:266:LEU:CG	2.30	0.80
1:A:265:ILE:O	1:A:268:GLU:CA	2.30	0.80
1:A:1004:PHE:CE1	1:A:1064:GLU:HG3	2.17	0.79
1:B:1050:ILE:HG23	1:B:1062:GLU:HG2	1.64	0.79
1:A:137:ALA:HB2	1:A:148:ARG:NE	1.97	0.78
1:A:265:ILE:HG22	1:A:266:LEU:H	1.49	0.76
1:A:267:LEU:O	1:A:268:GLU:HG2	1.84	0.76
1:A:137:ALA:CB	1:A:148:ARG:CZ	2.64	0.75
1:A:146:ARG:N	1:A:147:PRO:CD	2.50	0.75
1:A:1006:MET:CE	1:A:1161:TYR:CZ	2.70	0.75
1:A:144:SER:HA	1:A:147:PRO:HG3	1.69	0.74
1:B:60:ILE:CD1	1:B:85:LEU:HD22	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:HIS:HD2	1:B:161:TRP:HE1	1.35	0.73
1:B:208:LEU:HD22	1:B:256:TYR:CE1	2.23	0.72
1:A:1005:GLU:HA	1:A:1008:ARG:CB	2.20	0.72
1:B:262:ASP:HB2	1:B:280:VAL:CG1	2.20	0.71
1:B:1050:ILE:HG23	1:B:1062:GLU:CG	2.21	0.70
1:A:143:ASN:H	1:A:143:ASN:HD22	0.77	0.69
1:B:1005:GLU:OE2	1:B:230:LYS:HE2	1.91	0.69
1:A:1006:MET:CE	1:A:1161:TYR:CE2	2.76	0.69
1:B:259:ILE:O	1:B:263:SER:N	2.26	0.69
1:A:267:LEU:C	1:A:268:GLU:HG2	2.13	0.69
2:B:1500:ITD:H17	2:B:1500:ITD:S2	2.33	0.69
1:B:265:ILE:O	1:B:266:LEU:CB	2.40	0.68
1:A:180:ALA:HB2	1:A:185:ILE:HD12	1.76	0.68
1:B:266:LEU:HD12	1:B:266:LEU:C	2.14	0.67
1:A:70:ARG:HH21	1:A:75:LYS:HD3	1.59	0.65
1:A:265:ILE:O	1:A:268:GLU:N	2.30	0.64
1:B:265:ILE:O	1:B:265:ILE:HG22	1.95	0.64
1:B:1023:GLY:O	1:B:1024:TYR:CD2	2.51	0.64
1:A:180:ALA:CB	1:A:185:ILE:HD12	2.28	0.63
1:A:272:GLN:HG3	1:A:276:PHE:CD2	2.33	0.63
1:A:276:PHE:O	1:A:280:VAL:HG23	1.99	0.63
1:A:174:PHE:CD1	1:A:190:TYR:CE2	2.87	0.63
1:A:142:THR:OG1	1:A:143:ASN:N	2.30	0.62
1:A:1005:GLU:HA	1:A:1008:ARG:HB2	1.80	0.62
1:A:179:GLU:HG3	1:A:184:TYR:CE1	2.34	0.62
1:B:232:HIS:N	1:B:232:HIS:CD2	2.67	0.62
1:A:101:ASN:HD22	1:A:184:TYR:H	1.46	0.61
1:A:101:ASN:HB2	1:A:183:ARG:HB2	1.81	0.61
1:A:65:TYR:N	1:A:65:TYR:CD1	2.69	0.60
1:B:1005:GLU:HG3	1:B:230:LYS:HZ1	1.65	0.60
1:A:63:MET:CE	1:A:302:TYR:OH	2.49	0.60
1:A:144:SER:C	1:A:147:PRO:HD2	2.23	0.59
1:A:1004:PHE:CE1	1:A:1064:GLU:HA	2.37	0.59
1:A:225:LYS:HA	1:A:228:HIS:CE1	2.36	0.59
1:A:173:ILE:HG22	1:A:174:PHE:CA	2.32	0.58
1:B:1050:ILE:HD12	1:B:1062:GLU:CG	2.32	0.58
1:A:63:MET:HE1	1:A:302:TYR:OH	2.03	0.58
1:B:65:TYR:CD1	1:B:65:TYR:N	2.69	0.58
1:A:264:PHE:O	1:A:268:GLU:N	2.37	0.58
1:A:267:LEU:O	1:A:268:GLU:CG	2.52	0.57
1:A:144:SER:HA	1:A:147:PRO:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:MET:HG3	1:B:1161:TYR:CZ	2.39	0.57
1:A:1004:PHE:CE1	1:A:1064:GLU:CG	2.87	0.56
1:C:40:PHE:CE2	1:C:44:ILE:HD11	2.40	0.56
1:B:1022:GLU:HA	1:B:1022:GLU:OE1	2.04	0.56
1:A:144:SER:CA	1:A:147:PRO:HG3	2.35	0.56
1:A:1006:MET:HE3	1:A:1161:TYR:CE2	2.40	0.56
1:A:1005:GLU:HA	1:A:1008:ARG:HB3	1.87	0.56
1:A:144:SER:O	1:A:147:PRO:HG2	2.07	0.55
1:B:1005:GLU:HG3	1:B:230:LYS:NZ	2.20	0.55
1:C:1050:ILE:HD12	1:C:1062:GLU:HB3	1.89	0.54
1:B:1050:ILE:CG2	1:B:1062:GLU:HG2	2.36	0.54
1:A:66:GLN:HE22	1:B:224:SER:HB3	1.73	0.54
1:B:1061:ASP:N	1:B:1061:ASP:OD1	2.42	0.53
1:A:63:MET:HE2	1:A:302:TYR:CZ	2.43	0.53
1:A:101:ASN:CB	1:A:183:ARG:HB2	2.37	0.53
1:C:1019:LYS:HE3	1:C:1023:GLY:HA2	1.90	0.53
1:A:1006:MET:HE2	1:A:1161:TYR:CE2	2.40	0.52
1:A:273:GLY:O	1:A:275:GLU:N	2.43	0.52
1:C:267:LEU:C	1:C:268:GLU:CG	2.75	0.52
1:A:39:ILE:HG12	1:B:261:ILE:HD13	1.91	0.52
1:A:62:VAL:HG21	1:B:223:ILE:HD12	1.91	0.52
1:C:1007:LEU:HD13	1:C:1067:PHE:HZ	1.75	0.51
1:A:219:TYR:O	1:A:223:ILE:HG12	2.10	0.51
1:C:231:GLY:O	1:C:235:ARG:NH1	2.44	0.51
1:B:111:ALA:HA	1:B:114:VAL:HG22	1.93	0.51
1:A:273:GLY:O	1:A:274:CYS:C	2.49	0.50
1:A:1002:ASN:O	1:A:1158:TRP:CH2	2.63	0.50
1:C:187:ASP:HB3	2:C:1500:ITD:S2	2.52	0.50
1:C:159:GLY:O	1:C:163:PRO:HG2	2.11	0.50
1:A:146:ARG:H	1:A:147:PRO:CD	2.14	0.50
1:A:1004:PHE:HE1	1:A:1064:GLU:HA	1.77	0.50
1:A:70:ARG:NH2	1:A:75:LYS:HD3	2.25	0.49
1:A:181:ASP:N	1:A:181:ASP:OD1	2.45	0.49
1:B:116:TYR:CE2	2:B:1500:ITD:H3B	2.47	0.49
1:C:138:ILE:HG21	1:C:222:ILE:HG23	1.94	0.49
1:A:215:ILE:HG21	1:A:245:ILE:HG21	1.94	0.49
1:B:1005:GLU:OE2	1:B:230:LYS:CE	2.60	0.48
1:C:151:LEU:HA	1:C:155:VAL:HB	1.95	0.48
1:B:294:HIS:HA	1:B:297:LEU:HD12	1.95	0.48
1:A:174:PHE:CD1	1:A:190:TYR:HE2	2.30	0.48
1:A:134:ARG:O	1:A:138:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1157:THR:HA	1:B:232:HIS:CE1	2.48	0.48
1:C:1050:ILE:HG23	1:C:1062:GLU:HG2	1.95	0.48
1:B:88:VAL:HA	1:B:91:LEU:HD12	1.96	0.47
1:B:1091:LEU:HD22	1:B:1095:ARG:HB3	1.97	0.47
1:C:1161:TYR:N	1:C:1161:TYR:CD2	2.82	0.47
1:A:39:ILE:HG12	1:B:261:ILE:CD1	2.44	0.47
1:C:1020:ASP:OD2	1:C:1024:TYR:O	2.32	0.47
1:A:174:PHE:CD1	1:A:190:TYR:CD2	3.02	0.47
1:B:200:GLN:O	1:B:204:ILE:HG12	2.15	0.47
1:A:63:MET:O	1:A:64:GLY:C	2.53	0.47
1:B:265:ILE:O	1:B:266:LEU:HB3	2.13	0.47
1:C:97:ASP:CG	2:C:1500:ITD:H21	2.36	0.47
1:B:183:ARG:NH2	2:B:1500:ITD:H13A	2.31	0.46
1:A:63:MET:HE2	1:A:302:TYR:OH	2.16	0.46
1:A:174:PHE:HD1	1:A:190:TYR:HE2	1.64	0.46
1:A:1006:MET:CE	1:A:1161:TYR:OH	2.63	0.46
1:B:1006:MET:HG3	1:B:1161:TYR:CE1	2.50	0.46
1:A:163:PRO:HA	1:A:166:LEU:HD12	1.97	0.46
1:B:1021:THR:O	1:B:1021:THR:HG22	2.16	0.46
1:A:144:SER:CA	1:A:147:PRO:CG	2.93	0.46
1:B:151:LEU:HA	1:B:155:VAL:HB	1.98	0.46
1:B:63:MET:O	1:B:64:GLY:C	2.54	0.46
1:A:114:VAL:HG11	1:A:172:PHE:CE2	2.52	0.45
1:B:187:ASP:HB3	2:B:1500:ITD:S2	2.56	0.45
1:A:60:ILE:HD12	1:A:85:LEU:HD22	1.99	0.45
1:B:259:ILE:CG2	1:B:260:SER:N	2.49	0.45
1:A:97:ASP:OD1	2:A:1500:ITD:H15	2.17	0.44
1:A:1125:ARG:HB3	1:A:1128:GLU:HB2	1.98	0.44
1:A:173:ILE:CG2	1:A:174:PHE:N	2.51	0.44
1:A:143:ASN:ND2	1:A:143:ASN:N	2.30	0.44
1:B:262:ASP:OD1	1:B:262:ASP:O	2.35	0.44
1:A:114:VAL:HG11	1:A:172:PHE:CD2	2.53	0.44
1:B:1054:THR:HG21	1:B:1058:ILE:HG22	2.00	0.43
1:A:1005:GLU:H	1:A:1005:GLU:HG2	1.55	0.43
1:B:1050:ILE:HG23	1:B:1062:GLU:CD	2.38	0.43
1:A:228:HIS:CG	1:A:228:HIS:O	2.70	0.43
1:A:1016:LYS:HG3	1:A:1057:VAL:HG22	2.01	0.43
1:C:125:TRP:HB3	1:C:160:VAL:HG22	2.01	0.43
1:B:1157:THR:HA	1:B:232:HIS:NE2	2.34	0.43
1:A:144:SER:C	1:A:147:PRO:CD	2.87	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HG22	1:C:241:THR:HG23	2.01	0.42
1:A:144:SER:O	1:A:147:PRO:CG	2.67	0.42
1:A:65:TYR:N	1:A:65:TYR:HD1	2.16	0.42
2:C:1500:ITD:C17	2:C:1500:ITD:S2	3.07	0.42
1:B:210:LEU:HD21	1:C:210:LEU:HD11	2.01	0.42
1:B:261:ILE:HG22	1:B:262:ASP:CA	2.48	0.42
1:A:262:ASP:O	1:A:266:LEU:HD12	2.19	0.42
1:B:259:ILE:HG23	1:B:263:SER:CB	2.50	0.42
1:A:901:SER:C	1:A:1003:ILE:H	2.23	0.42
1:A:265:ILE:HG22	1:A:266:LEU:CA	2.42	0.42
1:A:273:GLY:C	1:A:275:GLU:N	2.74	0.41
1:B:1034:THR:HB	1:B:1045:GLU:HG3	2.02	0.41
1:C:1027:ILE:HG21	1:C:1046:LEU:HD13	2.01	0.41
1:A:1002:ASN:O	1:A:1158:TRP:CE3	2.69	0.41
1:A:190:TYR:HB3	1:A:195:TRP:HB2	2.02	0.41
1:A:102:TRP:HE1	1:A:109:CYS:HB2	1.84	0.41
1:B:70:ARG:CZ	1:B:78:LEU:HD21	2.50	0.41
1:C:88:VAL:HA	1:C:91:LEU:HD12	2.02	0.41
1:B:132:LEU:HA	1:B:218:CYS:SG	2.60	0.41
1:A:145:GLN:HG3	1:A:145:GLN:H	1.55	0.41
1:A:102:TRP:CH2	2:A:1500:ITD:H20	2.55	0.41
1:B:262:ASP:HA	1:B:265:ILE:HB	2.03	0.41
1:A:1094:VAL:HG22	1:A:1158:TRP:HE1	1.86	0.41
1:B:1124:LYS:HD3	1:B:1126:TRP:HZ2	1.86	0.41
1:A:272:GLN:HG3	1:A:276:PHE:HD2	1.80	0.40
1:B:65:TYR:N	1:B:65:TYR:HD1	2.15	0.40
1:B:259:ILE:C	1:B:263:SER:CB	2.90	0.40
2:C:1500:ITD:H18	2:C:1500:ITD:H3	2.01	0.40
1:C:85:LEU:HA	1:C:88:VAL:HG22	2.04	0.40
1:C:79:HIS:HD2	1:C:161:TRP:HE1	1.68	0.40
1:B:167:LEU:HD21	1:B:206:VAL:HG11	2.04	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	427/502 (85%)	395 (92%)	29 (7%)	3 (1%)	26	65
1	B	416/502 (83%)	394 (95%)	22 (5%)	0	100	100
1	C	418/502 (83%)	402 (96%)	15 (4%)	1 (0%)	52	84
All	All	1261/1506 (84%)	1191 (94%)	66 (5%)	4 (0%)	46	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1023	GLY
1	A	182	ASP
1	A	274	CYS
1	A	1077	GLY

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	368/432 (85%)	336 (91%)	32 (9%)	13	44
1	B	359/432 (83%)	328 (91%)	31 (9%)	13	45
1	C	365/432 (84%)	337 (92%)	28 (8%)	16	50
All	All	1092/1296 (84%)	1001 (92%)	91 (8%)	14	46

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	61	LEU
1	A	101	ASN
1	A	102	TRP
1	A	132	LEU
1	A	143	ASN

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Mol	Chain	Res	Type
1	A	144	SER
1	A	145	GLN
1	A	146	ARG
1	A	156	VAL
1	A	158	VAL
1	A	165	LEU
1	A	168	THR
1	A	171	ASP
1	A	181	ASP
1	A	186	CYS
1	A	187	ASP
1	A	228	HIS
1	A	901	SER
1	A	1005	GLU
1	A	1006	MET
1	A	1007	LEU
1	A	1083	LYS
1	A	1125	ARG
1	A	1132	ASN
1	A	1137	ARG
1	A	1141	GLN
1	A	232	HIS
1	A	265	ILE
1	A	266	LEU
1	A	269	ILE
1	A	277	GLU
1	B	38	LYS
1	B	39	ILE
1	B	53	ILE
1	B	69	LEU
1	B	79	HIS
1	B	81	SER
1	B	106	ASN
1	B	145	GLN
1	B	150	LEU
1	B	167	LEU
1	B	168	THR
1	B	172	PHE
1	B	183	ARG
1	B	186	CYS
1	B	205	MET
1	B	1008	ARG

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Mol	Chain	Res	Type
1	B	1016	LYS
1	B	1061	ASP
1	B	1062	GLU
1	B	1076	ARG
1	B	1085	LYS
1	B	1104	PHE
1	B	1106	MET
1	B	1201	SER
1	B	230	LYS
1	B	232	HIS
1	B	259	ILE
1	B	261	ILE
1	B	265	ILE
1	B	266	LEU
1	B	301	LEU
1	C	53	ILE
1	C	60	ILE
1	C	63	MET
1	C	69	LEU
1	C	81	SER
1	C	89	ILE
1	C	134	ARG
1	C	140	HIS
1	C	149	LYS
1	C	162	ILE
1	C	168	THR
1	C	200	GLN
1	C	225	LYS
1	C	1007	LEU
1	C	1020	ASP
1	C	1021	THR
1	C	1032	LEU
1	C	1035	LYS
1	C	1039	LEU
1	C	1047	ASP
1	C	1052	ARG
1	C	1137	ARG
1	C	239	LYS
1	C	245	ILE
1	C	246	LEU
1	C	265	ILE
1	C	266	LEU

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Mol	Chain	Res	Type
1	C	268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	101	ASN
1	A	143	ASN
1	A	1053	ASN
1	A	1055	ASN
1	A	272	GLN
1	B	79	HIS
1	B	119	ASN
1	B	232	HIS
1	B	294	HIS
1	C	66	GLN
1	C	203	HIS
1	C	272	GLN
1	C	294	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ITD	A	1500	-	25,30,30	2.03	5 (20%)	27,42,42	2.34	7 (25%)
2	ITD	B	1500	-	25,30,30	2.09	5 (20%)	27,42,42	2.06	10 (37%)
2	ITD	C	1500	-	25,30,30	2.08	5 (20%)	27,42,42	1.74	7 (25%)

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	ITD	A	1500	-	-	0/11/39/39	0/3/4/4
2	ITD	B	1500	-	-	0/11/39/39	0/3/4/4
2	ITD	C	1500	-	-	0/11/39/39	0/3/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1500	ITD	C9-S2	-8.00	1.66	1.75
2	B	1500	ITD	C9-S2	-7.89	1.66	1.75
2	A	1500	ITD	C9-S2	-7.52	1.67	1.75
2	A	1500	ITD	C2-N1	-3.20	1.46	1.49
2	B	1500	ITD	C2-N1	-2.93	1.46	1.49
2	C	1500	ITD	C2-N1	-2.47	1.47	1.49
2	A	1500	ITD	C8-S2	-2.06	1.76	1.82
2	C	1500	ITD	C8-S2	-2.04	1.76	1.82
2	B	1500	ITD	C8-S2	-2.03	1.76	1.82
2	A	1500	ITD	C5-S1	2.70	1.74	1.70
2	B	1500	ITD	C5-S1	3.05	1.74	1.70
2	C	1500	ITD	C5-S1	3.09	1.74	1.70
2	C	1500	ITD	C9-N4	3.95	1.34	1.26
2	B	1500	ITD	C9-N4	4.09	1.34	1.26
2	A	1500	ITD	C9-N4	4.17	1.34	1.26

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ITD	C7-C8-S2	-3.34	106.58	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1500	ITD	C7-C8-S2	-3.28	106.69	112.84
2	B	1500	ITD	C7-C8-S2	-2.73	107.73	112.84
2	B	1500	ITD	C3-C2-C6	-2.27	108.68	112.13
2	B	1500	ITD	C12-C11-C10	-2.07	107.93	111.13
2	B	1500	ITD	C11-C10-N3	2.19	114.61	110.56
2	C	1500	ITD	C11-C10-N3	2.22	114.66	110.56
2	C	1500	ITD	C17-C16-N4	2.37	113.11	109.33
2	C	1500	ITD	C10-N3-C9	2.80	129.33	124.86
2	A	1500	ITD	C6-C2-N1	3.03	105.80	102.85
2	C	1500	ITD	C16-N4-C9	3.04	125.94	121.07
2	B	1500	ITD	C6-C2-N1	3.07	105.84	102.85
2	C	1500	ITD	C6-C2-N1	3.19	105.96	102.85
2	B	1500	ITD	C17-C16-N4	3.21	114.47	109.33
2	B	1500	ITD	C10-N3-C9	3.67	130.71	124.86
2	B	1500	ITD	C8-S2-C9	3.76	106.04	99.53
2	C	1500	ITD	C8-S2-C9	3.97	106.40	99.53
2	B	1500	ITD	C16-N4-C9	4.21	127.81	121.07
2	A	1500	ITD	C16-N4-C9	4.27	127.91	121.07
2	B	1500	ITD	C15-C10-N3	4.37	118.64	110.56
2	A	1500	ITD	C15-C10-N3	4.40	118.70	110.56
2	A	1500	ITD	C17-C16-N4	4.46	116.46	109.33
2	A	1500	ITD	C10-N3-C9	4.48	132.02	124.86
2	A	1500	ITD	C8-S2-C9	6.20	110.25	99.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ITD	2	0
2	B	1500	ITD	4	0
2	C	1500	ITD	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	433/502 (86%)	0.02	15 (3%) 48 23	68, 89, 125, 161	0
1	B	426/502 (84%)	0.21	30 (7%) 19 7	63, 100, 181, 198	0
1	C	428/502 (85%)	0.13	19 (4%) 38 17	72, 98, 169, 207	0
All	All	1287/1506 (85%)	0.12	64 (4%) 32 13	63, 94, 169, 207	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	HIS	6.4
1	A	66	GLN	5.0
1	A	69	LEU	4.8
1	C	1037	PRO	4.7
1	C	29	PHE	4.7
1	B	27	PRO	4.6
1	B	1051	GLY	4.5
1	B	1057	VAL	4.0
1	B	1135	LYS	3.9
1	C	69	LEU	3.8
1	C	28	CYS	3.8
1	A	1002	ASN	3.7
1	C	1055	ASN	3.7
1	C	68	LYS	3.6
1	B	1037	PRO	3.6
1	C	1057	VAL	3.5
1	B	304	PHE	3.5
1	C	1024	TYR	3.5
1	B	1036	SER	3.5
1	C	27	PRO	3.4
1	C	145	GLN	3.3
1	A	1140	ASN	3.3
1	B	70	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1143	PRO	3.0
1	B	1038	SER	3.0
1	B	1049	ALA	2.8
1	C	230	LYS	2.8
1	B	272	GLN	2.8
1	B	65	TYR	2.8
1	B	1021	THR	2.8
1	B	262	ASP	2.7
1	A	67	LYS	2.7
1	B	1023	GLY	2.6
1	B	1136	SER	2.6
1	B	1201	SER	2.6
1	A	145	GLN	2.6
1	B	1011	GLU	2.6
1	C	173	ILE	2.5
1	B	1028	GLY	2.4
1	B	274	CYS	2.4
1	C	1048	LYS	2.4
1	C	1062	GLU	2.4
1	C	1036	SER	2.4
1	C	1033	LEU	2.4
1	A	100	ALA	2.3
1	C	1040	ASN	2.3
1	A	182	ASP	2.3
1	B	28	CYS	2.3
1	A	68	LYS	2.3
1	A	1125	ARG	2.2
1	B	69	LEU	2.2
1	B	33	ASN	2.2
1	C	1053	ASN	2.2
1	C	65	TYR	2.1
1	B	1026	THR	2.1
1	A	70	ARG	2.1
1	A	187	ASP	2.1
1	B	1012	GLY	2.1
1	B	1159	ASP	2.1
1	B	1141	GLN	2.0
1	A	179	GLU	2.0
1	A	181	ASP	2.0
1	B	1053	ASN	2.0
1	B	1035	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 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(\AA^2)	Q<0.9
2	ITD	A	1500	27/27	0.88	0.23	-0.20	37,105,187,191	0
2	ITD	C	1500	27/27	0.91	0.21	-0.25	35,105,168,218	0
2	ITD	B	1500	27/27	0.95	0.19	-0.28	24,89,203,224	0

6.5 Other polymers [i](#)

There are no such residues in this entry.