



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID : 3OE6
Title : Crystal structure of the CXCR4 chemokine receptor in complex with a small molecule antagonist IT1t in I222 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 : 3.20 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

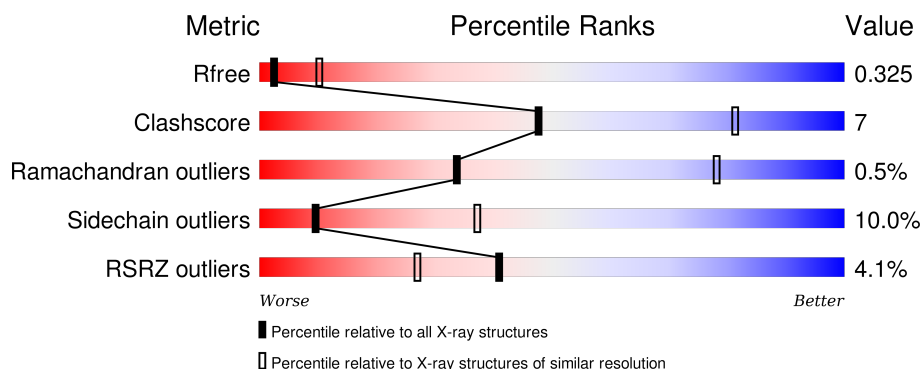
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	508	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3441 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.

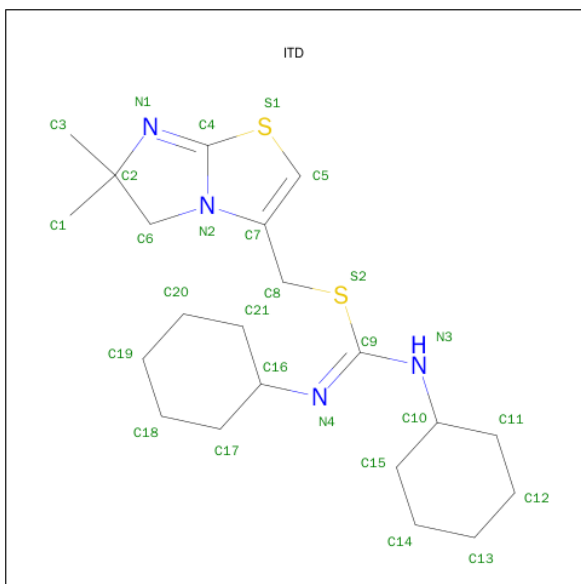
- Molecule 1 is a protein called C-X-C chemokine receptor type 4, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	1	0
			3362	2217	560	571	14			

There are 27 discrepancies between the modelled and reference sequences:

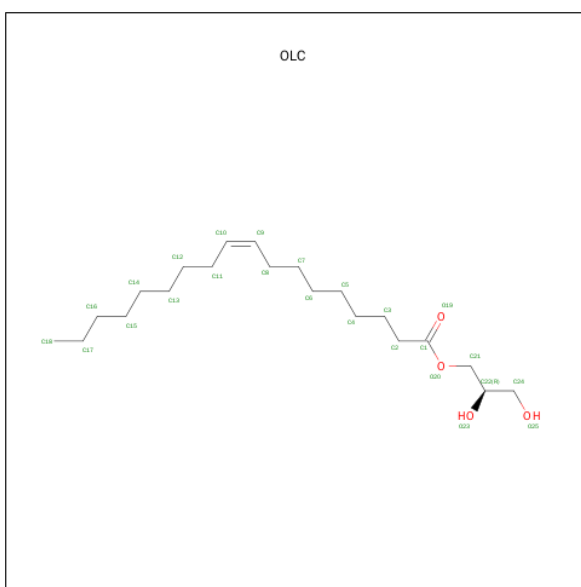
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
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	326	GLY	-	expression tag	UNP P61073
A	327	ARG	-	expression tag	UNP P61073
A	328	PRO	-	expression tag	UNP P61073
A	329	LEU	-	expression tag	UNP P61073
A	330	GLU	-	expression tag	UNP P61073
A	331	VAL	-	expression tag	UNP P61073
A	332	LEU	-	expression tag	UNP P61073
A	333	PHE	-	expression tag	UNP P61073
A	334	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: $C_{21}H_{34}N_4S_2$).



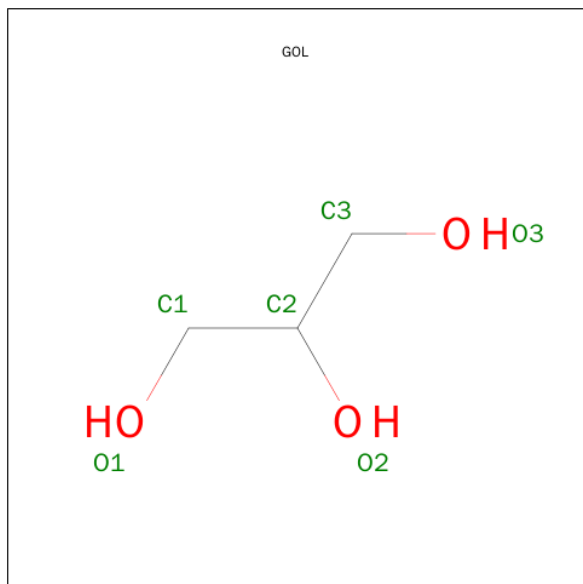
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			27	21	4	2		

- Molecule 3 is (2R)-2,3-DIHYDROXYPROPYL (9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		
3	A	1	Total	C	O	0	0
			15	11	4		
3	A	1	Total	C	O	0	0
			16	12	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	71.12Å 78.71Å 240.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20 6.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20) 85.7 (6.00-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.20Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.232 , 0.306 0.256 , 0.325	Depositor DCC
R_{free} test set	406 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.80 , 166.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 8310 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3441	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.80% 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: GOL, ITD, OLC

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	0.48	1/3446 (0.0%)	0.78	15/4677 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ASN	N-CA	5.07	1.56	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1092	ASP	CB-CA-C	-8.54	93.33	110.40
1	A	1093	ALA	CB-CA-C	-7.31	99.14	110.10
1	A	1083	LYS	CB-CA-C	7.25	124.89	110.40
1	A	100	ALA	N-CA-CB	-7.10	100.16	110.10
1	A	101	ASN	N-CA-CB	6.81	122.86	110.60
1	A	1093	ALA	N-CA-C	6.63	128.89	111.00
1	A	98	ALA	CB-CA-C	6.61	120.02	110.10
1	A	153	GLU	CB-CA-C	5.55	121.50	110.40
1	A	1108	GLU	CB-CA-C	-5.47	99.46	110.40
1	A	154	LYS	N-CA-CB	-5.35	100.98	110.60
1	A	100	ALA	N-CA-C	5.32	125.35	111.00
1	A	1155	THR	N-CA-C	5.25	125.16	111.00
1	A	1032	LEU	CB-CA-C	-5.22	100.28	110.20
1	A	99	VAL	CB-CA-C	5.17	121.23	111.40
1	A	1094	VAL	CB-CA-C	-5.10	101.72	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3362	0	3451	52	0
2	A	27	0	34	2	0
3	A	46	0	59	1	0
4	A	6	0	8	1	0
All	All	3441	0	3552	52	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 7.

All (52) 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:1078:ILE:HG23	1:A:1084:LEU:HD11	1.43	1.00
1:A:38:LYS:O	1:A:42:PRO:HG3	1.62	1.00
1:A:144:SER:O	1:A:147:PRO:HD2	1.62	0.99
1:A:1033:LEU:HG	1:A:1046:LEU:HD13	1.47	0.95
1:A:38:LYS:O	1:A:42:PRO:CG	2.15	0.94
1:A:146:ARG:HB2	1:A:147:PRO:HD3	1.58	0.85
1:A:1094:VAL:HG12	1:A:1095:ARG:N	1.96	0.80
1:A:180:ALA:CB	1:A:185:ILE:HD12	2.14	0.78
1:A:146:ARG:CB	1:A:147:PRO:HD3	2.12	0.78
1:A:186:CYS:SG	1:A:186:CYS:O	2.50	0.69
1:A:1092:ASP:O	1:A:1096:ARG:HB2	1.93	0.69
1:A:1078:ILE:HG23	1:A:1084:LEU:CD1	2.24	0.66
1:A:1094:VAL:HG11	1:A:1156:GLY:HA2	1.78	0.65
1:A:100:ALA:O	1:A:101:ASN:ND2	2.34	0.60
1:A:120:LEU:HG	4:A:1603:GOL:H32	1.83	0.59
1:A:146:ARG:HB2	1:A:147:PRO:CD	2.31	0.59
1:A:1155:THR:HG1	1:A:1158:TRP:HD1	1.51	0.59
1:A:187:ASP:HB3	2:A:1500:ITD:S2	2.43	0.58
1:A:243:ILE:HD11	1:A:301:LEU:HD21	1.85	0.58
1:A:1142:THR:HB	1:A:1145:ARG:HB2	1.87	0.57
1:A:146:ARG:CB	1:A:147:PRO:CD	2.81	0.56
1:A:1095:ARG:HG2	1:A:1153:PHE:HA	1.90	0.54
1:A:48:ILE:HD13	1:A:292:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:O	1:A:42:PRO:CD	2.57	0.52
1:A:1033:LEU:HG	1:A:1046:LEU:CD1	2.33	0.51
1:A:140:HIS:O	1:A:144:SER:HB3	2.10	0.51
1:A:1033:LEU:N	1:A:1033:LEU:HD12	2.27	0.49
1:A:1095:ARG:CG	1:A:1153:PHE:HA	2.43	0.49
1:A:117:THR:HB	1:A:168:THR:HG22	1.96	0.47
1:A:215:ILE:HG21	1:A:245:ILE:HG21	1.97	0.46
1:A:1081:ASN:HB3	1:A:1084:LEU:CD2	2.45	0.46
1:A:1087:VAL:O	1:A:1091:LEU:HG	2.16	0.45
1:A:102:TRP:NE1	1:A:109:CYS:HB2	2.32	0.45
1:A:145:GLN:HB2	1:A:145:GLN:HE21	1.67	0.44
1:A:62:VAL:HG11	3:A:1600:OLC:H21	2.00	0.44
1:A:144:SER:C	1:A:146:ARG:N	2.70	0.43
1:A:1033:LEU:H	1:A:1033:LEU:HD12	1.83	0.43
1:A:149:LYS:O	1:A:153:GLU:HG2	2.18	0.43
1:A:1097:ALA:HA	1:A:1100:ILE:HD12	2.01	0.42
1:A:127:LEU:HD23	1:A:130:ILE:HD12	2.01	0.42
1:A:145:GLN:O	1:A:145:GLN:HG3	2.19	0.42
1:A:144:SER:C	1:A:146:ARG:H	2.23	0.42
1:A:1142:THR:HB	1:A:1145:ARG:HD2	2.01	0.42
1:A:1027:ILE:HG22	1:A:1033:LEU:HD11	2.01	0.42
1:A:134:ARG:HD2	1:A:241:THR:HG21	2.00	0.42
1:A:1094:VAL:O	1:A:1094:VAL:HG13	2.20	0.41
1:A:97:ASP:OD1	2:A:1500:ITD:H16	2.20	0.41
1:A:1103:VAL:HG22	1:A:1111:VAL:HG21	2.01	0.41
1:A:268:GLU:HG2	1:A:271:LYS:HD3	2.04	0.40
1:A:72:MET:HG2	1:A:133:ASP:OD2	2.22	0.40
1:A:274:CYS:HA	1:A:277:GLU:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	411/508 (81%)	389 (95%)	20 (5%)	2 (0%)	34 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLY
1	A	147	PRO

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	360/437 (82%)	324 (90%)	36 (10%)	9 37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	67	LYS
1	A	72	MET
1	A	86	LEU
1	A	106	ASN
1	A	132	LEU
1	A	134	ARG
1	A	143	ASN
1	A	145	GLN
1	A	150	LEU
1	A	154	LYS
1	A	166	LEU
1	A	179	GLU
1	A	185	ILE
1	A	186	CYS
1	A	201	PHE
1	A	202	GLN
1	A	1014	ARG
1	A	1016	LYS

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Mol	Chain	Res	Type
1	A	1046	LEU
1	A	1057	VAL
1	A	1075	VAL
1	A	1080	ARG
1	A	1084	LEU
1	A	1095	ARG
1	A	1117	SER
1	A	1126	TRP
1	A	1132	ASN
1	A	1137	ARG
1	A	1138	TRP
1	A	1157	THR
1	A	235	ARG
1	A	243	ILE
1	A	246	LEU
1	A	300	ILE
1	A	311	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	1105	GLN
1	A	1132	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	2.04	6 (24%)	27,42,42	1.94	6 (22%)
3	OLC	A	1600	-	14,14,24	0.52	0	15,15,25	0.69	0
3	OLC	A	1601	-	14,14,24	0.51	0	15,15,25	0.68	0
3	OLC	A	1602	-	15,15,24	0.49	0	16,16,25	0.73	0
4	GOL	A	1603	-	5,5,5	0.32	0	5,5,5	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ITD	A	1500	-	-	0/11/39/39	0/3/4/4
3	OLC	A	1600	-	-	0/14/14/24	0/0/0/0
3	OLC	A	1601	-	-	0/14/14/24	0/0/0/0
3	OLC	A	1602	-	-	0/15/15/24	0/0/0/0
4	GOL	A	1603	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C9-S2	-7.87	1.66	1.75
2	A	1500	ITD	C2-N1	-2.65	1.46	1.49
2	A	1500	ITD	C8-S2	-2.14	1.76	1.82
2	A	1500	ITD	C4-N1	2.11	1.34	1.31
2	A	1500	ITD	C5-S1	2.58	1.74	1.70
2	A	1500	ITD	C9-N4	3.92	1.34	1.26

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1500	ITD	C7-C8-S2	-3.10	107.03	112.84
2	A	1500	ITD	C15-C10-N3	2.15	114.53	110.56
2	A	1500	ITD	C6-C2-N1	3.13	105.90	102.85
2	A	1500	ITD	C16-N4-C9	3.59	126.82	121.07
2	A	1500	ITD	C17-C16-N4	3.93	115.61	109.33
2	A	1500	ITD	C8-S2-C9	5.74	109.45	99.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ITD	2	0
3	A	1600	OLC	1	0
4	A	1603	GOL	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	418/508 (82%)	-0.04	17 (4%) 41 27	36, 62, 111, 130	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	ASP	4.5
1	A	1157	THR	3.9
1	A	1049	ALA	3.7
1	A	1119	ARG	3.1
1	A	35	ASN	2.9
1	A	1123	GLN	2.9
1	A	1055	ASN	2.8
1	A	1038	SER	2.7
1	A	1072	ASP	2.7
1	A	142	THR	2.6
1	A	1054	THR	2.5
1	A	182	ASP	2.4
1	A	1059	THR	2.4
1	A	1155	THR	2.3
1	A	1053	ASN	2.2
1	A	1159	ASP	2.1
1	A	1046	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ITD	A	1500	27/27	0.93	0.20	0.50	16,65,145,189	0
4	GOL	A	1603	6/6	0.95	0.15	-0.02	59,60,60,61	0
3	OLC	A	1602	16/25	0.91	0.21	-0.30	35,78,131,153	0
3	OLC	A	1600	15/25	0.96	0.13	-0.77	3,47,111,134	0
3	OLC	A	1601	15/25	0.92	0.18	-1.15	29,62,84,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.