



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GMN
Title : CRYSTAL STRUCTURES OF NK1-HEPARIN COMPLEXES REVEAL THE BASIS FOR NK1 ACTIVITY AND ENABLE ENGINEERING OF POTENT AGONISTS OF THE MET RECEPTOR
Authors : Lietha, D.; Chirgadze, D.Y.; Mulloy, B.; Blundell, T.L.; Gherardi, E.
Deposited on : 2001-09-19
Resolution : 2.30 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

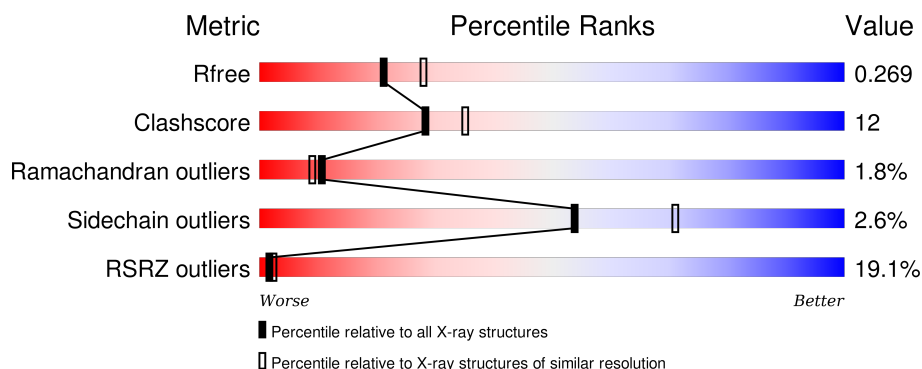
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	183	
1	B	183	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2353 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 HEPATOCYTE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1301	828	228	234	11			
1	B	113	Total	C	N	O	S	0	0	0
			869	549	147	165	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
A	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
B	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
B	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	5	Total	C	N	O	S	3	0
			86	30	2	47	7		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

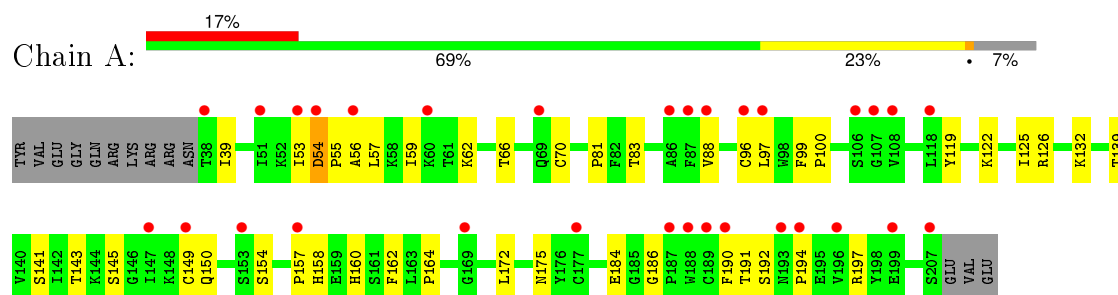
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	35	Total	O	0	0
			35	35		

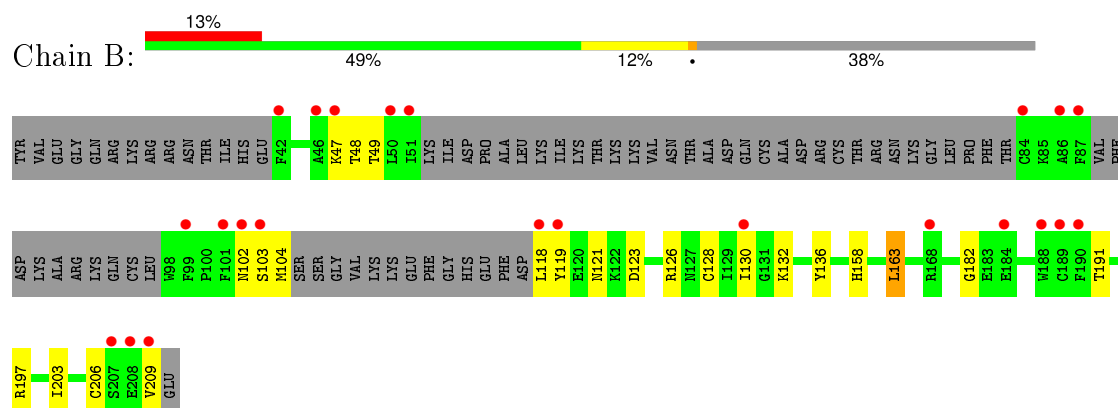
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: HEPATOCYTE GROWTH FACTOR



• Molecule 1: HEPATOCYTE GROWTH FACTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.56 Å 86.56 Å 117.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.30 20.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (21.00-2.30) 99.6 (20.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.30 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.279 0.269 , 0.269	Depositor DCC
R_{free} test set	1040 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20312 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2353	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: EPE, IDS, SGN

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	0.40	1/1335 (0.1%)	0.57	0/1801
1	B	0.39	0/891	0.58	0/1201
All	All	0.40	1/2226 (0.0%)	0.58	0/3002

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	GLU	CB-CG	-5.13	1.42	1.52

There are no bond angle outliers.

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	1301	0	1242	37	0
1	B	869	0	791	15	0
2	A	86	0	31	1	0
3	A	15	0	17	0	0
3	B	15	0	17	0	0
4	A	32	0	0	1	0
4	B	35	0	0	0	0
All	All	2353	0	2098	51	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 12.

All (51) 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:158:HIS:CD2	1:A:197:ARG:HA	2.13	0.84
1:B:128:CYS:HG	1:B:206:CYS:HG	0.85	0.83
1:A:154:SER:HB3	4:A:2025:HOH:O	1.84	0.77
1:A:88:VAL:HG23	1:A:99:PHE:HE2	1.54	0.73
1:A:160:HIS:HD2	1:A:162:PHE:H	1.35	0.73
1:A:70:CYS:SG	1:A:96:CYS:HB2	2.30	0.72
1:A:158:HIS:NE2	1:A:197:ARG:HA	2.04	0.71
1:A:126:ARG:HH22	1:B:209:VAL:HG22	1.56	0.71
1:A:70:CYS:HG	1:A:96:CYS:HB2	1.57	0.70
1:A:160:HIS:CD2	1:A:162:PHE:H	2.10	0.69
1:A:122:LYS:HE2	1:A:139:THR:HG21	1.75	0.68
1:A:59:ILE:HD12	1:A:99:PHE:HD1	1.58	0.67
1:A:96:CYS:C	1:A:97:LEU:HD12	2.18	0.64
1:B:163:LEU:HD23	1:B:163:LEU:N	2.14	0.63
1:A:57:LEU:HD13	1:A:100:PRO:HG3	1.83	0.61
1:A:70:CYS:HG	1:A:96:CYS:CB	2.13	0.60
1:A:57:LEU:HD13	1:A:100:PRO:CG	2.32	0.59
1:B:48:THR:HG22	1:B:49:THR:H	1.67	0.59
1:A:70:CYS:SG	1:A:96:CYS:SG	3.01	0.58
1:B:136:TYR:CZ	1:B:203:ILE:HD13	2.39	0.58
1:A:141:SER:HB2	1:A:175:ASN:ND2	2.19	0.58
1:A:157:PRO:HG2	1:A:158:HIS:ND1	2.20	0.56
1:B:48:THR:HG22	1:B:49:THR:N	2.22	0.55
1:A:160:HIS:CD2	1:A:162:PHE:HB2	2.43	0.54
1:A:160:HIS:HD2	1:A:162:PHE:N	2.04	0.54
1:B:102:ASN:C	1:B:104:MET:H	2.11	0.53
1:A:160:HIS:HD2	1:A:162:PHE:HB2	1.73	0.53
1:B:158:HIS:CE1	1:B:197:ARG:HA	2.45	0.52
1:B:102:ASN:O	1:B:104:MET:N	2.44	0.50
1:A:70:CYS:SG	1:A:96:CYS:CB	3.00	0.50
1:A:53:ILE:O	1:A:54:ASP:HB3	2.13	0.49
1:A:62:LYS:HE2	2:A:1212:IDS:O2S	2.13	0.48
1:B:121:ASN:ND2	1:B:123:ASP:HB2	2.30	0.47
1:A:192:SER:O	1:A:194:PRO:HD3	2.15	0.46
1:A:70:CYS:HB3	1:A:96:CYS:SG	2.56	0.46
1:B:102:ASN:C	1:B:104:MET:N	2.69	0.45
1:A:88:VAL:CG2	1:A:99:PHE:HE2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HG3	1:A:172:LEU:O	2.16	0.45
1:B:163:LEU:CD2	1:B:163:LEU:N	2.80	0.44
1:A:143:THR:C	1:A:145:SER:H	2.21	0.44
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.83	0.43
1:A:160:HIS:CD2	1:A:162:PHE:N	2.83	0.43
1:A:97:LEU:HD12	1:A:97:LEU:N	2.34	0.43
1:A:132:LYS:O	1:A:186:GLY:HA2	2.19	0.42
1:B:126:ARG:HH12	1:B:130:ILE:HD12	1.85	0.42
1:A:39:ILE:HD11	1:A:119:TYR:CE2	2.55	0.41
1:A:149:CYS:HB2	1:A:175:ASN:HD22	1.85	0.41
1:B:132:LYS:HD3	1:B:182:GLY:O	2.20	0.41
1:B:118:LEU:HD12	1:B:119:TYR:N	2.36	0.41
1:A:125:ILE:O	1:A:126:ARG:C	2.60	0.40
1:A:150:GLN:N	1:A:190:PHE:O	2.48	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	168/183 (92%)	151 (90%)	14 (8%)	3 (2%)	11	9
1	B	105/183 (57%)	97 (92%)	6 (6%)	2 (2%)	10	8
All	All	273/366 (75%)	248 (91%)	20 (7%)	5 (2%)	11	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	PRO
1	A	56	ALA
1	B	103	SER
1	B	47	LYS

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Mol	Chain	Res	Type
1	A	81	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/165 (82%)	132 (97%)	4 (3%)	50	66
1	B	93/165 (56%)	91 (98%)	2 (2%)	60	77
All	All	229/330 (69%)	223 (97%)	6 (3%)	54	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	66	THR
1	A	83	THR
1	A	191	THR
1	B	163	LEU
1	B	191	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	160	HIS
1	A	175	ASN
1	B	158	HIS

5.3.3 RNA [i](#)

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 ⓘ

5 carbohydrates 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	IDS	A	1208	2	13,17,17	1.05	2 (15%)	19,26,26	4.35	4 (21%)
2	SGN	A	1209	2	17,19,20	1.01	1 (5%)	19,29,31	1.77	4 (21%)
2	IDS	A	1210	2	13,16,17	1.33	2 (15%)	17,24,26	1.62	4 (23%)
2	SGN	A	1211	2	17,19,20	1.21	2 (11%)	19,29,31	2.08	5 (26%)
2	IDS	A	1212	2	12,15,17	1.66	4 (33%)	12,22,26	0.91	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	IDS	A	1208	2	-	0/5/29/29	0/1/1/1
2	SGN	A	1209	2	-	0/11/28/31	0/1/1/1
2	IDS	A	1210	2	-	0/5/26/29	0/1/1/1
2	SGN	A	1211	2	-	0/11/28/31	0/1/1/1
2	IDS	A	1212	2	-	0/5/22/29	1/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1212	IDS	O2-C2	-3.30	1.42	1.47
2	A	1210	IDS	O2-C2	-3.30	1.42	1.47
2	A	1208	IDS	O2-C2	-2.05	1.42	1.46
2	A	1212	IDS	C4-C3	2.00	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1208	IDS	C4-C5	2.13	1.58	1.53
2	A	1209	SGN	C1-C2	2.15	1.55	1.52
2	A	1211	SGN	O2S-S1	2.29	1.44	1.42
2	A	1210	IDS	C1-C2	2.39	1.55	1.51
2	A	1211	SGN	C1-C2	2.44	1.55	1.52
2	A	1212	IDS	C1-C2	2.45	1.55	1.51
2	A	1212	IDS	C4-C5	2.62	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1211	SGN	O4-C4-C3	-3.94	101.46	110.34
2	A	1209	SGN	O4-C4-C3	-3.71	101.98	110.34
2	A	1209	SGN	O1S-S1-N	-3.30	104.09	108.50
2	A	1208	IDS	O4-C4-C3	-3.21	103.12	110.34
2	A	1211	SGN	O1S-S1-N	-3.04	104.44	108.50
2	A	1210	IDS	O4-C4-C3	-2.97	103.65	110.34
2	A	1211	SGN	C4-C3-C2	-2.13	107.92	111.23
2	A	1210	IDS	C4-C3-C2	2.14	113.92	110.20
2	A	1208	IDS	C1-O5-C5	2.31	115.63	112.22
2	A	1209	SGN	C1-O5-C5	2.68	115.64	112.25
2	A	1210	IDS	C1-O5-C5	2.98	116.43	111.84
2	A	1211	SGN	C1-O5-C5	3.33	116.48	112.25
2	A	1209	SGN	O4-C4-C5	3.87	119.50	109.24
2	A	1210	IDS	C1-C2-C3	4.13	115.54	109.39
2	A	1208	IDS	C2-O2-S	4.70	127.72	118.77
2	A	1211	SGN	O4-C4-C5	5.70	124.36	109.24
2	A	1208	IDS	O4-C4-C5	17.75	143.83	110.42

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1212	IDS	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1212	IDS	1	0

5.6 Ligand geometry

2 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	$\# Z > 2$
3	EPE	A	1213	-	14,15,15	1.18	1 (7%)	18,20,20	0.99	0
3	EPE	B	1210	-	14,15,15	1.08	1 (7%)	18,20,20	2.35	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	1213	-	-	0/9/19/19	0/1/1/1
3	EPE	B	1210	-	-	0/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1210	EPE	C6-N1	2.26	1.53	1.46
3	A	1213	EPE	C6-N1	2.34	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1210	EPE	O1S-S-C10	-7.81	100.25	106.91
3	B	1210	EPE	O2S-S-C10	5.27	111.41	106.91

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

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	170/183 (92%)	1.07	31 (18%) 2 3	35, 56, 77, 94	0
1	B	113/183 (61%)	1.13	23 (20%) 1 2	24, 47, 105, 110	0
All	All	283/366 (77%)	1.09	54 (19%) 2 2	24, 54, 99, 110	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	9.9
1	A	53	ILE	6.4
1	B	119	TYR	6.3
1	A	56	ALA	6.2
1	B	99	PHE	4.9
1	B	101	PHE	4.9
1	B	208	GLU	4.9
1	A	196	VAL	4.9
1	A	88	VAL	4.8
1	A	96	CYS	4.6
1	A	188	TRP	4.3
1	A	87	PHE	4.1
1	B	50	LEU	3.9
1	A	51	ILE	3.9
1	B	84	CYS	3.9
1	B	87	PHE	3.8
1	B	47	LYS	3.7
1	A	38	THR	3.5
1	B	168	ARG	3.4
1	A	86	ALA	3.3
1	B	184	GLU	3.3
1	A	189	CYS	3.2
1	A	169	GLY	3.0
1	A	149	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	3.0
1	B	86	ALA	3.0
1	A	177	CYS	3.0
1	A	69	GLN	2.9
1	B	190	PHE	2.9
1	A	107	GLY	2.9
1	A	190	PHE	2.8
1	A	207	SER	2.8
1	A	147	ILE	2.8
1	B	46	ALA	2.7
1	B	188	TRP	2.7
1	B	102	ASN	2.6
1	A	54	ASP	2.5
1	A	118	LEU	2.5
1	A	97	LEU	2.4
1	A	108	VAL	2.4
1	A	157	PRO	2.4
1	A	60	LYS	2.3
1	B	42	PHE	2.3
1	A	187	PRO	2.2
1	A	106	SER	2.2
1	B	207	SER	2.2
1	A	193	ASN	2.2
1	B	130	ILE	2.1
1	A	153	SER	2.1
1	A	194	PRO	2.1
1	B	51	ILE	2.1
1	B	189	CYS	2.0
1	B	103	SER	2.0
1	B	118	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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	IDS	A	1210	16/17	0.88	0.22	0.37	73,77,85,85	0
2	SGN	A	1209	19/20	0.89	0.18	-0.56	56,67,71,72	0
2	IDS	A	1208	17/17	0.78	0.28	-	73,94,102,102	3
2	IDS	A	1212	15/17	0.82	0.34	-	95,97,99,100	0
2	SGN	A	1211	19/20	0.91	0.17	-	84,86,88,93	0

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
3	EPE	B	1210	15/15	0.94	0.22	0.38	30,46,50,50	0
3	EPE	A	1213	15/15	0.91	0.23	0.19	63,64,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.