Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 09:17 PM EDT

PDB ID	:	2B4S
Title	:	Crystal structure of a complex between PTP1B and the insulin receptor tyrosine kinase
Authors	:	Li, S.; Depetris, R.S.; Barford, D.; Chernoff, J.; Hubbard, S.R.
Deposited on	:	2005-09-26
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
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:

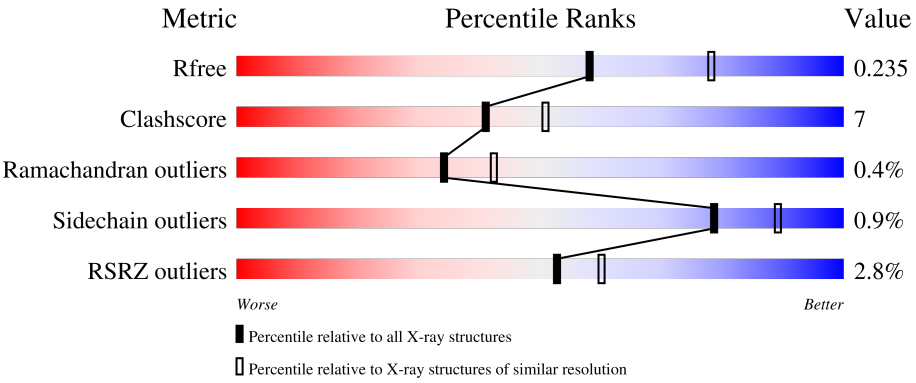
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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 <=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	298	3% 84% 12%
1	C	298	2% 74% 18% 7%
2	B	306	3% 78% 18%
2	D	306	3% 82% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9641 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 Tyrosine-protein phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2306	1465	399	429	13			
1	C	278	Total	C	N	O	S	0	0	0
			2244	1428	390	413	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	ALA	CYS	engineered mutation	UNP P18031
C	215	ALA	CYS	engineered mutation	UNP P18031

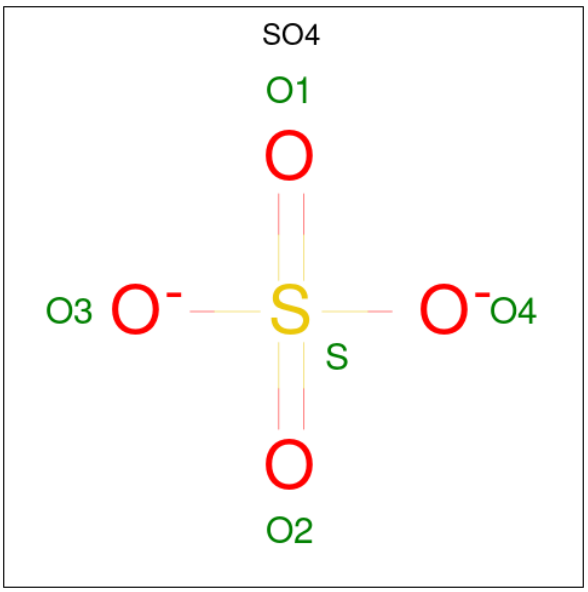
- Molecule 2 is a protein called Insulin receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	297	Total	C	N	O	P	S	0	0	0
			2326	1468	394	442	3	19			
2	D	297	Total	C	N	O	P	S	0	0	0
			2338	1474	399	443	3	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	981	SER	CYS	engineered mutation	UNP P06213
B	1158	PTR	TYR	modified residue	UNP P06213
B	1162	PTR	TYR	modified residue	UNP P06213
B	1163	PTR	TYR	modified residue	UNP P06213
B	1251	ASN	LYS	variant	UNP P06213
D	981	SER	CYS	engineered mutation	UNP P06213
D	1158	PTR	TYR	modified residue	UNP P06213
D	1162	PTR	TYR	modified residue	UNP P06213
D	1163	PTR	TYR	modified residue	UNP P06213
D	1251	ASN	LYS	variant	UNP P06213

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0

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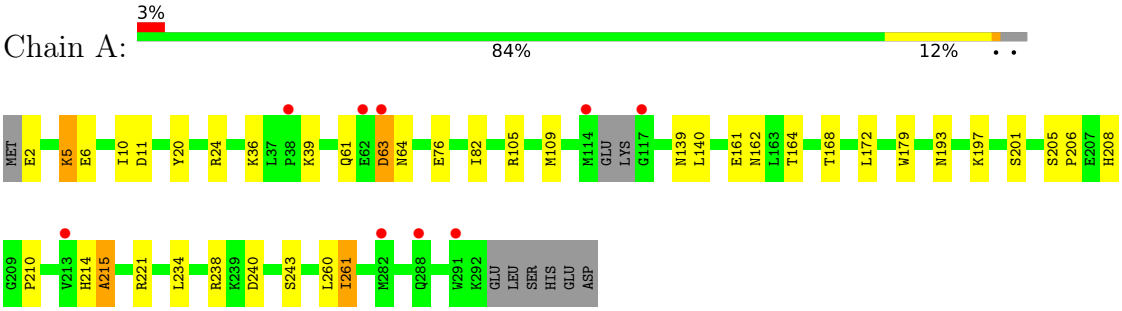
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	88	Total O 88 88	0	0
4	C	89	Total O 89 89	0	0
4	D	103	Total O 103 103	0	0

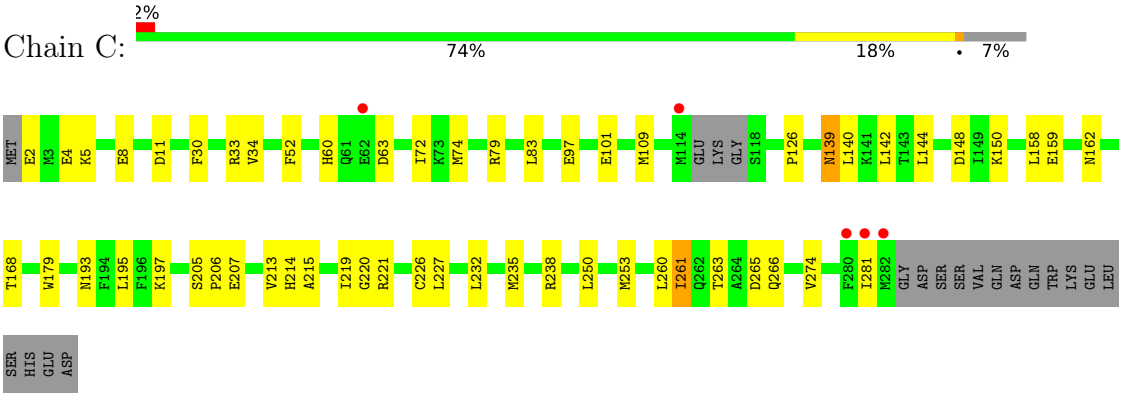
3 Residue-property plots (i)

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.

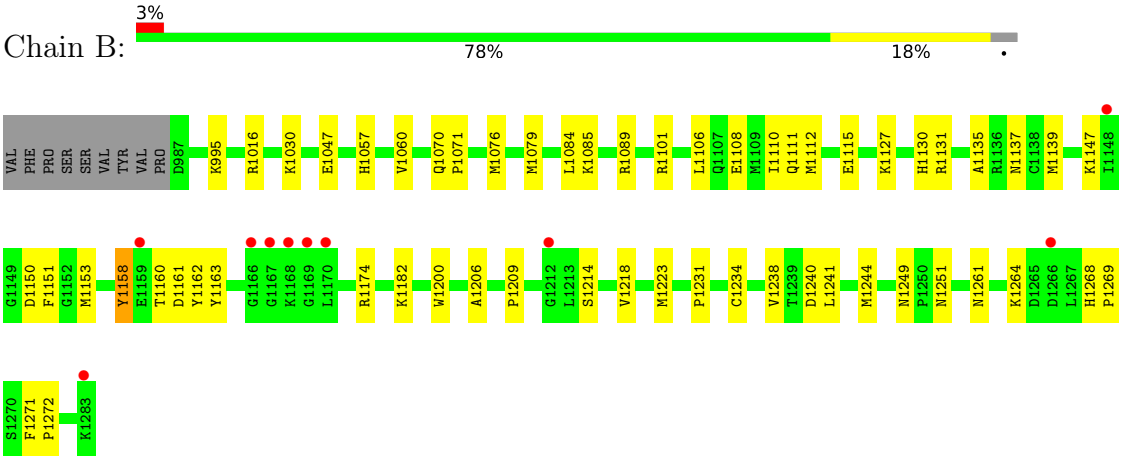
• Molecule 1: Tyrosine-protein phosphatase, non-receptor type 1



• Molecule 1: Tyrosine-protein phosphatase, non-receptor type 1

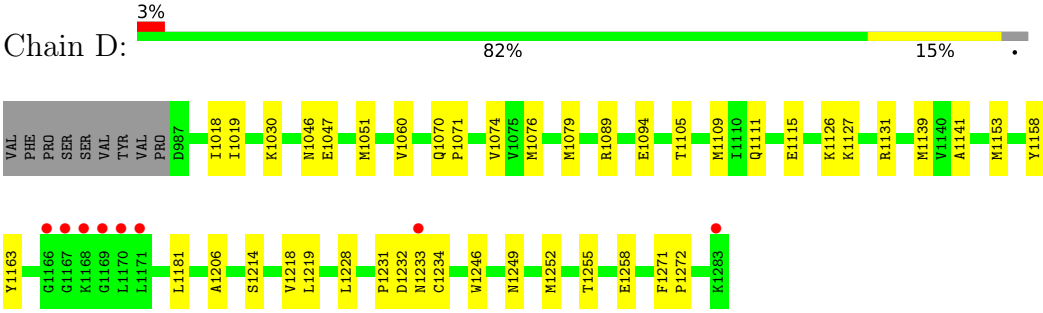


• Molecule 2: Insulin receptor



• Molecule 2: Insulin receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.47Å 88.17Å 178.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.30 29.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.49-2.30) 94.4 (29.49-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.62 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.239 0.202 , 0.235	Depositor DCC
R_{free} test set	2946 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9641	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1145e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PTR

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	0.36	0/2359	0.59	0/3190
1	C	0.37	0/2295	0.59	0/3099
2	B	0.36	0/2326	0.59	0/3149
2	D	0.36	0/2338	0.60	0/3163
All	All	0.36	0/9318	0.59	0/12601

There are no bond length outliers.

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	2306	0	2229	26	0
1	C	2244	0	2200	40	0
2	B	2326	0	2227	35	0
2	D	2338	0	2247	27	0
3	A	25	0	0	1	0
3	B	5	0	0	0	0
3	C	20	0	0	1	0
4	A	97	0	0	1	0
4	B	88	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	89	0	0	3	0
4	D	103	0	0	3	0
All	All	9641	0	8903	128	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 (128) 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)
2:D:1231:PRO:HG2	2:D:1234:CYS:HB2	1.62	0.79
1:C:232:LEU:HA	1:C:235:MET:HE3	1.65	0.78
2:D:1233:ASN:HA	4:D:209:HOH:O	1.86	0.75
1:C:250:LEU:HD13	1:C:261:ILE:HD12	1.74	0.70
2:D:1070:GLN:HE21	2:D:1071:PRO:HA	1.58	0.69
1:C:232:LEU:HD23	1:C:235:MET:HE1	1.76	0.68
1:A:238:ARG:HD3	1:A:243:SER:OG	1.96	0.66
2:B:1089:ARG:HG3	2:B:1206:ALA:HB3	1.78	0.65
1:C:232:LEU:HD23	1:C:235:MET:CE	2.29	0.63
2:B:1127:LYS:HG3	2:B:1158:PTR:HD1	1.80	0.63
1:C:250:LEU:CD1	1:C:261:ILE:HD12	2.28	0.63
2:B:1108:GLU:O	2:B:1112:MET:HG3	1.99	0.62
1:A:6:GLU:O	1:A:10:ILE:HG13	2.00	0.61
1:A:61:GLN:HE21	1:A:63:ASP:HB2	1.66	0.61
2:B:1182:LYS:HB2	2:B:1223:MET:HE3	1.83	0.59
1:C:227:LEU:HD22	1:C:261:ILE:HD11	1.83	0.59
2:B:1106:LEU:O	2:B:1110:ILE:HG12	2.02	0.59
2:D:1131:ARG:HD3	2:D:1153:MET:O	2.03	0.59
2:D:1070:GLN:NE2	2:D:1071:PRO:HA	2.19	0.58
2:D:1018:ILE:HG13	2:D:1019:ILE:HG13	1.86	0.57
1:C:60:HIS:HB2	1:C:101:GLU:OE2	2.05	0.57
1:A:5:LYS:HD2	1:A:6:GLU:N	2.19	0.57
1:A:109:MET:HG3	1:A:214:HIS:CE1	2.41	0.56
1:C:235:MET:CE	1:C:274:VAL:HG13	2.35	0.56
2:B:1070:GLN:NE2	2:B:1071:PRO:HA	2.21	0.56
1:C:30:PHE:HB2	1:C:52:PHE:CD2	2.41	0.56
2:B:1200:TRP:CD1	2:B:1231:PRO:HD3	2.41	0.56
2:B:1231:PRO:HG2	2:B:1234:CYS:HB2	1.89	0.55
1:C:97:GLU:O	1:C:101:GLU:HG3	2.07	0.55
2:D:1051:MET:SD	2:D:1076:MET:HE3	2.47	0.54
1:C:126:PRO:HD3	1:C:142:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1131:ARG:HD3	2:B:1153:MET:O	2.08	0.53
1:C:235:MET:HE2	1:C:274:VAL:HG13	1.90	0.53
2:B:1241:LEU:HD23	2:B:1244:MET:HE1	1.89	0.53
1:C:263:THR:OG1	1:C:266:GLN:HG3	2.09	0.53
1:A:2:GLU:O	1:A:5:LYS:HG3	2.09	0.52
2:D:1181:LEU:HD22	2:D:1219:LEU:HD23	1.91	0.52
2:D:1232:ASP:O	2:D:1233:ASN:CG	2.48	0.52
1:C:159:GLU:HG3	1:C:168:THR:HG23	1.92	0.51
1:C:215:ALA:HB3	3:C:1002:SO4:O3	2.10	0.51
2:D:1160:THR:O	2:D:1161:ASP:HB2	2.10	0.51
1:C:193:ASN:O	1:C:197:LYS:HG2	2.10	0.51
1:A:105:ARG:HD2	1:A:208:HIS:NE2	2.25	0.51
2:B:1240:ASP:O	2:B:1244:MET:HG3	2.11	0.51
1:C:260:LEU:O	1:C:261:ILE:HB	2.10	0.51
1:C:83:LEU:HD23	1:C:213:VAL:HB	1.93	0.50
2:B:1111:GLN:O	2:B:1115:GLU:HG3	2.12	0.50
2:D:1255:THR:HG23	2:D:1258:GLU:OE2	2.11	0.50
2:D:1271:PHE:HB3	2:D:1272:PRO:HD3	1.92	0.50
2:B:995:LYS:HG2	2:B:1016:ARG:HE	1.77	0.49
1:C:238:ARG:HG3	4:C:1090:HOH:O	2.11	0.49
2:D:1089:ARG:HG3	2:D:1206:ALA:HB3	1.93	0.49
2:D:1111:GLN:O	2:D:1115:GLU:HG3	2.13	0.49
2:D:1219:LEU:C	2:D:1219:LEU:HD13	2.33	0.49
1:A:140:LEU:HD23	1:A:162:ASN:HA	1.95	0.49
2:B:1241:LEU:HD23	2:B:1244:MET:CE	2.43	0.48
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.49	0.48
2:B:1047:GLU:HG3	2:B:1151:PHE:HB2	1.96	0.48
1:A:61:GLN:HE21	1:A:64:ASN:H	1.62	0.47
2:B:1261:ASN:O	2:B:1264:LYS:HG2	2.15	0.47
1:C:179:TRP:CE2	1:C:221:ARG:HG2	2.50	0.47
1:C:219:ILE:HG13	1:C:220:GLY:N	2.30	0.47
2:B:1085:LYS:HE3	2:B:1089:ARG:CZ	2.46	0.46
1:C:72:ILE:HD11	1:C:83:LEU:HD12	1.96	0.46
1:A:39:LYS:HE3	4:A:1050:HOH:O	2.15	0.46
1:A:61:GLN:NE2	1:A:63:ASP:HB2	2.29	0.46
2:B:1268:HIS:CG	2:B:1269:PRO:HD2	2.50	0.46
2:D:1070:GLN:NE2	4:D:38:HOH:O	2.48	0.45
2:B:1057:HIS:O	2:B:1147:LYS:HE2	2.17	0.45
2:B:1214:SER:O	2:B:1218:VAL:HG23	2.16	0.45
2:D:1249:ASN:HD22	2:D:1252:MET:HG2	1.81	0.45
2:B:1130:HIS:O	2:B:1131:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HD2	1:A:5:LYS:C	2.36	0.45
2:B:1174:ARG:HB3	2:B:1209:PRO:HB2	1.99	0.45
1:A:260:LEU:O	1:A:261:ILE:HB	2.17	0.45
2:D:1079:MET:HG3	2:D:1139:MET:CB	2.46	0.45
2:B:1084:LEU:HB3	2:B:1135:ALA:O	2.17	0.44
2:D:1105:THR:O	2:D:1109:MET:HG3	2.18	0.44
2:B:1137:ASN:HB3	2:B:1150:ASP:HB3	1.98	0.44
1:A:139:ASN:HD22	1:A:164:THR:HG1	1.63	0.44
2:B:1271:PHE:HB3	2:B:1272:PRO:HD3	1.97	0.44
1:A:215:ALA:HB3	3:A:1000:SO4:O1	2.18	0.44
2:D:1228:LEU:HB2	2:D:1246:TRP:CH2	2.53	0.44
2:B:1249:ASN:ND2	2:B:1251:ASN:OD1	2.51	0.44
1:C:140:LEU:HD23	1:C:162:ASN:HA	2.00	0.44
1:C:205:SER:HA	1:C:206:PRO:HD3	1.81	0.44
2:D:1047:GLU:O	2:D:1051:MET:HG3	2.18	0.44
2:D:1214:SER:O	2:D:1218:VAL:HG23	2.18	0.43
2:B:1030:LYS:HE3	2:B:1076:MET:CE	2.49	0.43
1:A:105:ARG:HD2	1:A:208:HIS:CD2	2.54	0.43
1:A:161:GLU:HG3	1:A:168:THR:HG22	1.99	0.43
1:A:205:SER:HA	1:A:206:PRO:HD3	1.88	0.43
1:C:74:MET:HB3	4:C:1080:HOH:O	2.18	0.42
2:B:1084:LEU:HD11	2:B:1112:MET:HE1	2.00	0.42
2:B:1182:LYS:HB2	2:B:1223:MET:CE	2.48	0.42
1:A:193:ASN:O	1:A:197:LYS:HG2	2.18	0.42
1:C:179:TRP:NE1	1:C:221:ARG:HG2	2.35	0.42
1:A:172:LEU:CD1	1:A:201:SER:HB2	2.50	0.42
1:C:227:LEU:HD22	1:C:261:ILE:CD1	2.48	0.42
2:D:1060:VAL:HG12	2:D:1076:MET:HE2	2.01	0.42
1:A:76:GLU:HG2	1:A:234:LEU:CD2	2.49	0.42
2:D:1126:LYS:O	2:D:1127:LYS:HB2	2.20	0.42
2:B:1070:GLN:HE21	2:B:1071:PRO:HA	1.82	0.42
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.80	0.41
2:B:1160:THR:O	2:B:1161:ASP:HB2	2.19	0.41
2:B:1238:VAL:O	2:B:1241:LEU:HB2	2.20	0.41
2:D:1046:ASN:HB2	4:D:120:HOH:O	2.20	0.41
1:C:74:MET:SD	1:C:253:MET:HG2	2.60	0.41
1:C:144:LEU:HA	1:C:158:LEU:HD23	2.02	0.41
1:C:4:GLU:O	1:C:8:GLU:HG3	2.20	0.41
1:C:250:LEU:HD13	1:C:261:ILE:CD1	2.48	0.41
1:C:265:ASP:HB2	4:C:1027:HOH:O	2.19	0.41
2:B:1060:VAL:HG21	2:B:1139:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:LYS:HA	2:B:1223:MET:HE1	2.01	0.41
1:A:82:ILE:HG13	1:A:210:PRO:HB2	2.02	0.41
1:A:179:TRP:NE1	1:A:221:ARG:HG2	2.35	0.41
1:C:83:LEU:HD21	1:C:226:CYS:SG	2.60	0.41
2:D:1079:MET:HE3	2:D:1141:ALA:N	2.35	0.41
1:C:148:ASP:OD2	1:C:150:LYS:HE2	2.21	0.41
1:C:281:ILE:HG12	1:C:281:ILE:O	2.21	0.41
1:A:238:ARG:HG2	1:A:240:ASP:H	1.85	0.40
1:C:33:ARG:HH21	1:C:34:VAL:HG22	1.86	0.40
1:C:109:MET:HG3	1:C:214:HIS:CE1	2.56	0.40
1:C:139:ASN:HD22	1:C:139:ASN:HA	1.68	0.40
1:C:232:LEU:HA	1:C:235:MET:CE	2.44	0.40
2:D:1030:LYS:HB2	2:D:1074:VAL:HB	2.03	0.40
2:B:1079:MET:HG3	2:B:1139:MET:HB3	2.03	0.40
1:C:2:GLU:O	1:C:5:LYS:HG2	2.20	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	285/298 (96%)	276 (97%)	6 (2%)	3 (1%)	14 15
1	C	274/298 (92%)	268 (98%)	4 (2%)	2 (1%)	22 26
2	B	292/306 (95%)	285 (98%)	7 (2%)	0	100 100
2	D	292/306 (95%)	282 (97%)	10 (3%)	0	100 100
All	All	1143/1208 (95%)	1111 (97%)	27 (2%)	5 (0%)	34 42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	C	63	ASP
1	C	261	ILE
1	A	215	ALA
1	A	261	ILE

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	248/270 (92%)	246 (99%)	2 (1%)	81	91
1	C	244/270 (90%)	239 (98%)	5 (2%)	55	72
2	B	244/265 (92%)	243 (100%)	1 (0%)	91	96
2	D	246/265 (93%)	245 (100%)	1 (0%)	91	96
All	All	982/1070 (92%)	973 (99%)	9 (1%)	78	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	11	ASP
2	B	1101	ARG
1	C	11	ASP
1	C	79	ARG
1	C	139	ASN
1	C	195	LEU
1	C	207	GLU
2	D	1094	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	127	GLN
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	166	GLN
2	B	1014	ASN
2	B	1070	GLN
2	B	1081	HIS
2	B	1208	GLN
1	C	60	HIS
1	C	78	GLN
1	C	139	ASN
2	D	1004	GLN
2	D	1033	ASN
2	D	1070	GLN
2	D	1251	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	PTR	B	1163	2	15,16,17	0.85	0	19,22,24	1.02	3 (15%)
2	PTR	D	1163	2	15,16,17	1.17	1 (6%)	19,22,24	1.11	1 (5%)
2	PTR	D	1162	2	15,16,17	0.86	0	19,22,24	0.96	1 (5%)
2	PTR	B	1158	2	15,16,17	0.96	1 (6%)	19,22,24	0.90	1 (5%)
2	PTR	D	1158	2	15,16,17	1.13	1 (6%)	19,22,24	0.94	1 (5%)
2	PTR	B	1162	2	15,16,17	1.33	2 (13%)	19,22,24	0.91	1 (5%)

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	PTR	B	1163	2	-	0/10/11/13	0/1/1/1
2	PTR	D	1163	2	-	0/10/11/13	0/1/1/1
2	PTR	D	1162	2	-	1/10/11/13	0/1/1/1
2	PTR	B	1158	2	-	0/10/11/13	0/1/1/1
2	PTR	D	1158	2	-	0/10/11/13	0/1/1/1
2	PTR	B	1162	2	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1162	PTR	P-OH	3.88	1.65	1.59
2	D	1163	PTR	P-OH	3.66	1.64	1.59
2	D	1158	PTR	P-OH	3.18	1.64	1.59
2	B	1158	PTR	P-OH	2.41	1.63	1.59
2	B	1162	PTR	P-O2P	-2.16	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1163	PTR	P-OH-CZ	3.16	133.89	123.75
2	B	1162	PTR	P-OH-CZ	2.44	131.56	123.75
2	D	1162	PTR	P-OH-CZ	2.43	131.54	123.75
2	B	1163	PTR	O2P-P-OH	-2.31	98.03	105.24
2	B	1163	PTR	P-OH-CZ	2.26	131.00	123.75
2	D	1158	PTR	P-OH-CZ	2.25	130.96	123.75
2	B	1158	PTR	O3P-P-O2P	2.08	115.60	107.64
2	B	1163	PTR	O3P-P-O2P	2.01	115.33	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1162	PTR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1158	PTR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	SO4	A	1004	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	C	1002	-	4,4,4	0.20	0	6,6,6	0.18	0
3	SO4	A	1000	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SO4	C	1003	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	1009	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	C	1005	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	1284	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	A	1007	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	A	1008	-	4,4,4	0.29	0	6,6,6	0.06	0
3	SO4	A	1001	-	4,4,4	0.26	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	SO4	1	0
3	A	1000	SO4	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

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, 95^{th} 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	289/298 (96%)	0.00	9 (3%) 49 56	11, 21, 44, 51	0
1	C	278/298 (93%)	-0.10	5 (1%) 68 74	10, 20, 33, 49	0
2	B	294/306 (96%)	0.08	10 (3%) 45 52	12, 24, 38, 52	0
2	D	294/306 (96%)	0.12	8 (2%) 54 62	13, 24, 38, 63	0
All	All	1155/1208 (95%)	0.03	32 (2%) 53 60	10, 22, 39, 63	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1169	GLY	9.8
2	D	1168	LYS	7.9
2	D	1167	GLY	7.6
2	D	1166	GLY	6.8
2	D	1170	LEU	6.6
1	A	63	ASP	5.1
2	B	1166	GLY	5.0
2	B	1167	GLY	4.9
2	B	1168	LYS	4.1
1	C	281	ILE	4.1
1	C	62	GLU	4.0
2	B	1283	LYS	3.9
2	D	1283	LYS	3.9
2	B	1169	GLY	3.7
2	B	1170	LEU	3.3
1	C	282	MET	3.0
1	A	117	GLY	2.9
1	A	213	VAL	2.7
1	C	280	PHE	2.7
1	A	282	MET	2.7
2	B	1266	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLN	2.6
2	D	1233	ASN	2.6
1	C	114	MET	2.5
1	A	114	MET	2.4
2	B	1148	ILE	2.4
1	A	291	TRP	2.4
2	B	1212	GLY	2.3
1	A	38	PRO	2.3
1	A	62	GLU	2.2
2	B	1159	GLU	2.2
2	D	1171	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PTR	D	1158	16/17	0.78	0.27	36,47,57,58	0
2	PTR	B	1158	16/17	0.79	0.27	34,47,58,58	0
2	PTR	D	1162	16/17	0.90	0.19	36,38,42,42	0
2	PTR	D	1163	16/17	0.90	0.16	37,42,48,49	0
2	PTR	B	1163	16/17	0.92	0.14	35,37,43,43	0
2	PTR	B	1162	16/17	0.92	0.17	32,33,34,34	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	1008	5/5	0.85	0.26	72,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	1009	5/5	0.92	0.14	60,61,61,61	0
3	SO4	B	1284	5/5	0.96	0.14	40,40,41,41	0
3	SO4	A	1007	5/5	0.97	0.15	52,52,53,53	0
3	SO4	C	1003	5/5	0.97	0.12	40,40,41,42	0
3	SO4	A	1001	5/5	0.97	0.10	37,37,38,38	0
3	SO4	C	1002	5/5	0.99	0.12	12,14,14,15	0
3	SO4	A	1004	5/5	0.99	0.10	14,15,17,17	0
3	SO4	C	1005	5/5	0.99	0.09	13,13,13,14	0
3	SO4	A	1000	5/5	0.99	0.13	15,16,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.