Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2025 – 09:48 PM JST

PDB ID	:	21BJ / pdb_000021bj
Title	:	SHP2-PD1 Complex
Deposited on	:	2025-12-06
Resolution	:	2.61 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

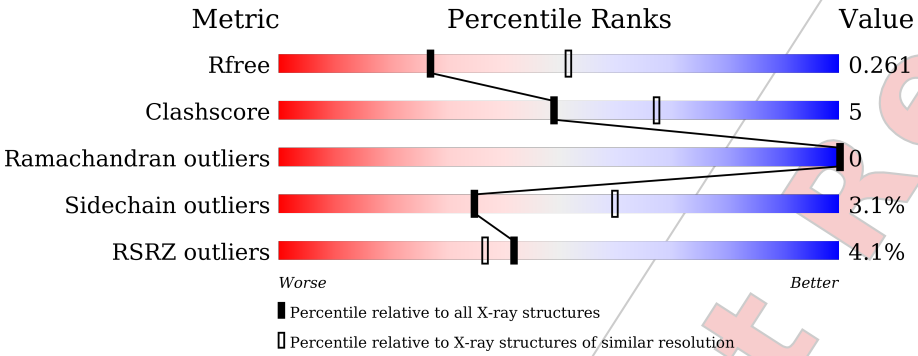
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.47

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 2.61 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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	525	4% 78% 17%
1	B	525	4% 83% 13% 5%
2	C	37	41% 11% 49%
2	D	37	5% 51% 8% 41%
3	E	4	25% 25% 50% 25%

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Mol	Chain	Length	Quality of chain
4	F	4	50% 75% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8422 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 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	501	Total	C	N	O	S	0	0	0
			3982	2506	708	752	16			
1	A	502	Total	C	N	O	S	0	0	0
			4032	2541	714	760	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	459	SER	CYS	engineered mutation	UNP Q06124
A	459	SER	CYS	engineered mutation	UNP Q06124

- Molecule 2 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	P	0	0	0
			183	113	23	45	2			
2	C	19	Total	C	N	O	P	0	0	0
			157	99	19	37	2			

- Molecule 3 is a protein called ALA-ALA-PTR-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	P	0	0	0
			31	18	4	8	1			

- Molecule 4 is a protein called ALA-PTR-ALA-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	P	0	0	0
			31	18	4	8	1			

- Molecule 5 is water.

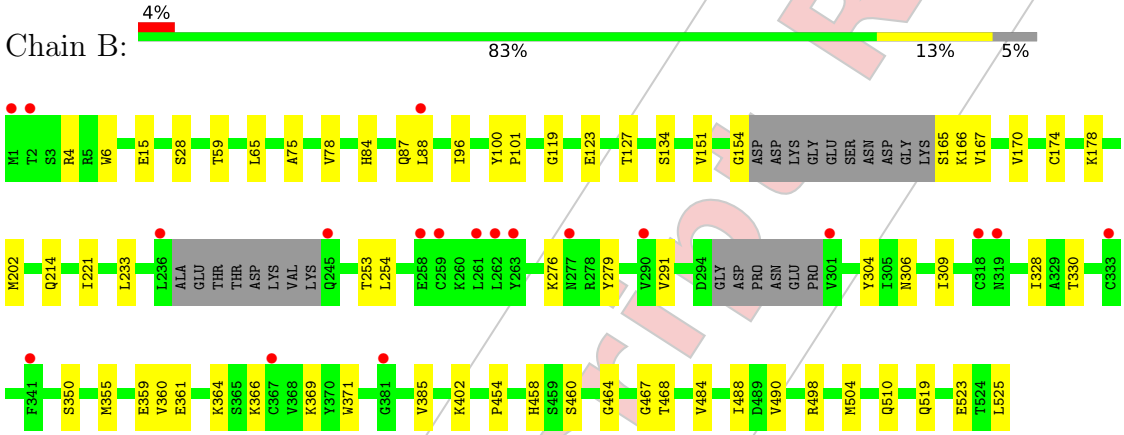
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total O 2 2	0	0
5	A	3	Total O 3 3	0	0
5	C	1	Total O 1 1	0	0

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.

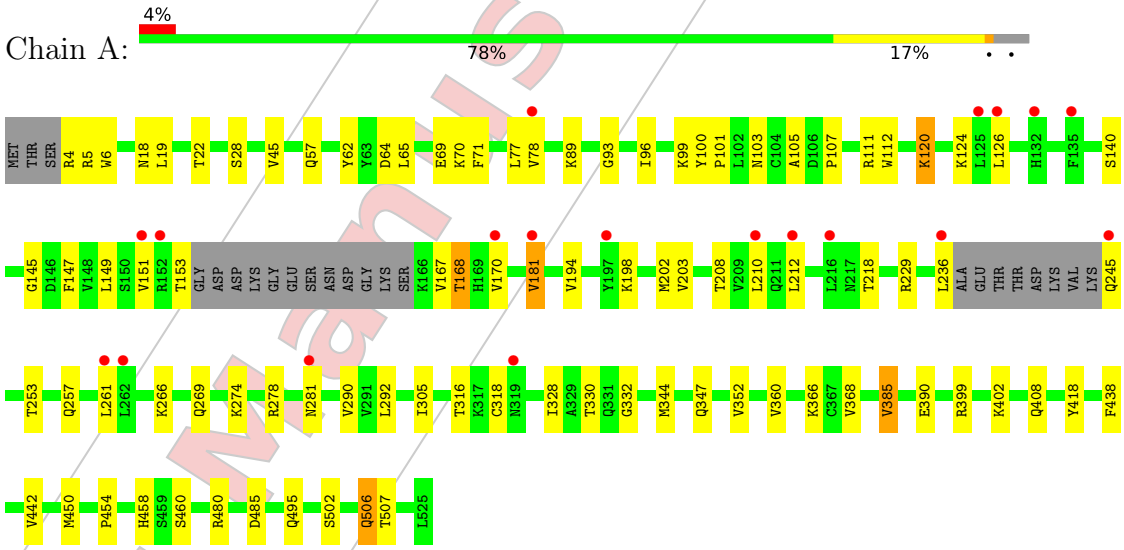
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 11

Chain B:



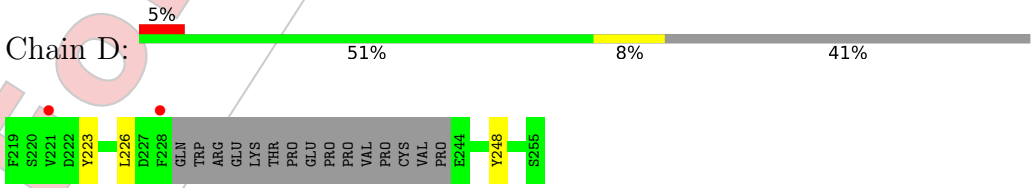
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 11

Chain A:



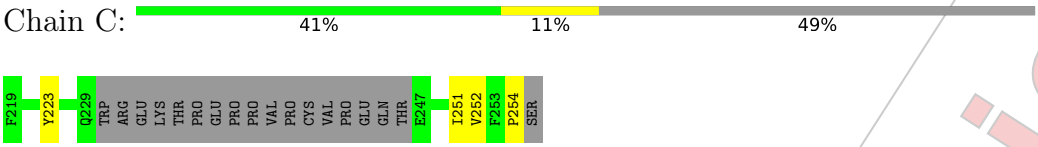
• Molecule 2: Programmed cell death protein 1

Chain D:



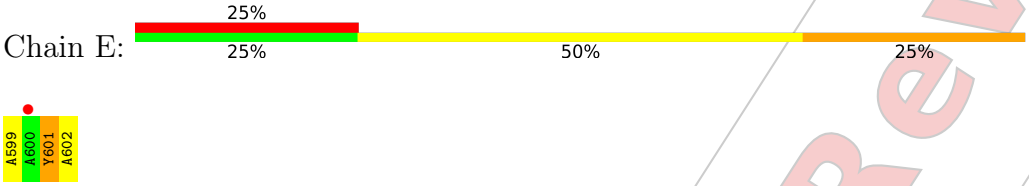
• Molecule 2: Programmed cell death protein 1

Chain C:



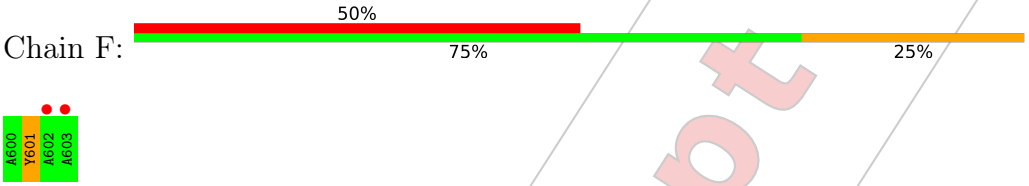
• Molecule 3: ALA-ALA-PTR-ALA

Chain E:



• Molecule 4: ALA-PTR-ALA-ALA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.38Å 107.73Å 216.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.28 – 2.61 31.28 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.5 (31.28-2.61) 97.7 (31.28-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.231 , 0.261 0.231 , 0.261	Depositor DCC
R_{free} test set	2408 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8422	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/4118	0.61	0/5565
1	B	0.38	0/4065	0.64	0/5498
2	C	0.36	0/124	0.60	0/164
2	D	0.48	0/150	0.70	0/199
3	E	0.29	0/13	0.18	0/15
4	F	0.22	0/13	0.34	0/15
All	All	0.38	0/8483	0.63	0/11456

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4032	0	3938	52	0
1	B	3982	0	3844	38	0
2	C	157	0	121	2	0
2	D	183	0	145	1	0
3	E	31	0	21	3	0
4	F	31	0	21	2	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	1	0	0	0	0
All	All	8422	0	8090	88	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 5.

All (88) 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:181:VAL:HG21	1:A:202:MET:SD	2.36	0.66
1:B:123:GLU:HG2	1:B:167:VAL:HG21	1.77	0.65
1:A:506:GLN:OE1	3:E:599:ALA:N	2.29	0.65
1:B:154:GLY:HA3	1:B:165:SER:HA	1.78	0.64
1:A:290:VAL:HG11	1:A:344:MET:HG3	1.82	0.62
1:B:170:VAL:HG21	1:B:202:MET:HE1	1.80	0.62
1:A:305:ILE:HD13	1:A:344:MET:HE2	1.84	0.60
1:B:484:VAL:HG11	1:A:105:ALA:HB2	1.83	0.59
1:A:149:LEU:HD11	1:A:212:LEU:HD11	1.84	0.58
1:A:28:SER:HA	1:A:100:TYR:O	2.05	0.57
1:A:236:LEU:HA	1:A:245:GLN:HA	1.85	0.57
1:A:111:ARG:HD3	1:A:229:ARG:NH2	2.20	0.56
1:A:408:GLN:N	1:A:408:GLN:OE1	2.39	0.56
1:B:123:GLU:O	1:B:127:THR:HG23	2.06	0.56
1:A:4:ARG:O	1:A:4:ARG:HG3	2.05	0.55
1:A:253:THR:O	1:A:257:GLN:HG2	2.07	0.55
1:A:278:ARG:NH2	1:A:332:GLY:O	2.40	0.55
1:B:355:MET:HE1	1:B:371:TRP:CZ3	2.44	0.53
1:A:316:THR:HG23	1:A:318:CYS:H	1.72	0.53
1:A:328:ILE:HG13	1:A:454:PRO:HB2	1.91	0.53
1:B:467:GLY:HA3	1:B:504:MET:O	2.09	0.52
1:B:464:GLY:O	1:B:468:THR:HG23	2.09	0.52
1:B:88:LEU:HD23	1:B:96:ILE:HB	1.93	0.51
1:A:112:TRP:CZ2	1:A:194:VAL:HG21	2.45	0.51
1:B:519:GLN:O	1:B:523:GLU:HG3	2.11	0.51
1:B:328:ILE:HG13	1:B:454:PRO:HB2	1.93	0.50
1:B:119:GLY:O	1:B:123:GLU:HG3	2.10	0.50
1:B:330:THR:HG23	1:B:458:HIS:HB3	1.93	0.50
1:B:525:LEU:HD11	1:A:19:LEU:HD22	1.94	0.50
1:B:309:ILE:HD13	1:B:328:ILE:HG12	1.94	0.50
1:B:65:LEU:HD13	2:D:226:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:CE1	1:A:70:LYS:HD3	2.48	0.49
1:B:28:SER:HA	1:B:100:TYR:O	2.11	0.49
1:A:57:GLN:N	1:A:64:ASP:O	2.42	0.48
1:A:450:MET:HA	1:A:450:MET:HE3	1.95	0.48
1:B:306:ASN:HD22	1:B:306:ASN:C	2.21	0.48
1:A:292:LEU:HD11	1:A:305:ILE:HB	1.96	0.48
1:A:6:TRP:HB3	1:A:101:PRO:HB3	1.96	0.48
1:B:361:GLU:HG3	1:B:366:LYS:HG3	1.95	0.48
1:B:385:VAL:HA	1:B:402:LYS:O	2.14	0.47
1:A:316:THR:C	1:A:318:CYS:H	2.22	0.47
1:B:134:SER:HA	1:B:214:GLN:O	2.15	0.47
1:B:460:SER:HB3	4:F:601:PTR:O3P	2.15	0.47
2:C:252:VAL:O	2:C:254:PRO:HD3	2.16	0.46
1:A:460:SER:HB3	3:E:601:PTR:O2P	2.15	0.46
1:B:279:TYR:CE2	4:F:601:PTR:HB3	2.50	0.46
1:B:4:ARG:HG3	1:B:4:ARG:O	2.16	0.46
1:B:498:ARG:HG2	1:B:504:MET:H	1.80	0.46
1:B:221:ILE:HG23	1:B:488:ILE:HG13	1.98	0.45
1:A:385:VAL:HA	1:A:402:LYS:O	2.16	0.45
1:A:18:ASN:O	1:A:22:THR:HG23	2.17	0.45
1:B:174:CYS:HA	1:B:178:LYS:O	2.16	0.45
1:A:261:LEU:HD11	1:A:495:GLN:OE1	2.16	0.45
1:B:6:TRP:HB3	1:B:101:PRO:HB3	1.98	0.44
1:A:390:GLU:HG2	1:A:399:ARG:HG2	2.00	0.44
1:A:4:ARG:NH2	1:A:145:GLY:H	2.14	0.44
1:B:350:SER:OG	1:B:454:PRO:O	2.25	0.44
1:A:194:VAL:O	1:A:198:LYS:HB2	2.18	0.44
1:A:352:VAL:HG11	1:A:442:VAL:HG13	2.00	0.44
1:B:84:HIS:HB3	1:B:87:GLN:HG3	1.99	0.44
1:A:418:TYR:HB3	1:A:438:PHE:CE1	2.52	0.44
1:A:274:LYS:HD2	1:A:274:LYS:HA	1.58	0.43
1:A:330:THR:HG23	1:A:458:HIS:HB3	2.01	0.43
1:A:281:ASN:OD1	3:E:602:ALA:HB3	2.19	0.43
1:B:276:LYS:HD2	1:B:304:TYR:HD2	1.82	0.43
1:B:15:GLU:OE2	1:A:480:ARG:HD3	2.18	0.43
1:A:203:VAL:HG13	2:C:252:VAL:HB	2.01	0.43
1:A:6:TRP:CH2	1:A:78:VAL:HG11	2.54	0.42
1:A:107:PRO:HG3	1:A:147:PHE:CE2	2.55	0.42
1:B:6:TRP:CH2	1:B:75:ALA:HA	2.55	0.42
1:B:6:TRP:CZ2	1:B:75:ALA:HA	2.55	0.42
1:A:5:ARG:HE	1:A:103:ASN:CG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG11	1:A:96:ILE:HG21	2.01	0.42
1:A:120:LYS:O	1:A:124:LYS:HG2	2.20	0.42
1:A:278:ARG:HH22	1:A:332:GLY:C	2.27	0.42
1:A:111:ARG:NH1	1:A:218:THR:O	2.52	0.41
1:A:168:THR:HG21	1:A:210:LEU:HD21	2.02	0.41
1:A:99:LYS:HB2	1:A:100:TYR:CD1	2.54	0.41
1:A:65:LEU:HD21	1:A:77:LEU:HD21	2.02	0.41
1:A:198:LYS:HG2	1:A:212:LEU:O	2.20	0.41
1:B:468:THR:CG2	1:B:510:GLN:HB3	2.50	0.41
1:B:359:GLU:OE2	1:B:369:LYS:HB2	2.21	0.41
1:A:266:LYS:HE3	1:A:269:GLN:OE1	2.21	0.41
1:A:69:GLU:HB3	1:A:71:PHE:CE1	2.55	0.40
1:A:292:LEU:HA	1:A:347:GLN:OE1	2.21	0.40
1:B:170:VAL:HG11	1:B:202:MET:HE1	2.04	0.40
1:B:360:VAL:HG13	1:B:364:LYS:C	2.47	0.40
1:A:89:LYS:HE3	1:A:93:GLY:HA2	2.04	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	496/525 (94%)	476 (96%)	20 (4%)	0	100	100
1	B	493/525 (94%)	475 (96%)	18 (4%)	0	100	100
2	C	13/37 (35%)	12 (92%)	1 (8%)	0	100	100
2	D	16/37 (43%)	16 (100%)	0	0	100	100
3	E	1/4 (25%)	0	1 (100%)	0	100	100
4	F	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1020/1132 (90%)	980 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	439/467 (94%)	421 (96%)	18 (4%)	26	49
1	B	426/467 (91%)	417 (98%)	9 (2%)	48	72
2	C	13/33 (39%)	12 (92%)	1 (8%)	10	21
2	D	17/33 (52%)	17 (100%)	0	100	100
All	All	895/1000 (90%)	867 (97%)	28 (3%)	35	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	THR
1	B	78	VAL
1	B	151	VAL
1	B	166	LYS
1	B	233	LEU
1	B	253	THR
1	B	254	LEU
1	B	291	VAL
1	B	490	VAL
1	A	120	LYS
1	A	126	LEU
1	A	140	SER
1	A	151	VAL
1	A	153	THR
1	A	167	VAL
1	A	168	THR
1	A	170	VAL
1	A	181	VAL
1	A	208	THR
1	A	360	VAL
1	A	366	LYS
1	A	368	VAL

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Mol	Chain	Res	Type
1	A	385	VAL
1	A	485	ASP
1	A	502	SER
1	A	506	GLN
1	A	507	THR
2	C	251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	HIS
1	B	196	HIS
1	B	257	GLN
1	B	287	HIS
1	B	293	HIS
1	B	306	ASN
1	B	347	GLN
1	B	506	GLN
1	B	510	GLN
1	B	520	HIS
1	A	37	ASN
1	A	143	HIS
1	A	196	HIS
1	A	200	ASN
1	A	222	ASN
1	A	271	GLN
1	A	293	HIS
1	A	298	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	223	2	15,16,17	1.23	1 (6%)	19,22,24	0.78	0
2	PTR	D	248	2	15,16,17	1.26	1 (6%)	19,22,24	0.89	0
2	PTR	C	248	2	15,16,17	0.50	0	19,22,24	0.59	0
2	PTR	D	223	2	15,16,17	1.24	1 (6%)	19,22,24	0.75	1 (5%)
3	PTR	E	601	3	15,16,17	1.22	2 (13%)	19,22,24	0.69	1 (5%)
4	PTR	F	601	4	15,16,17	1.21	1 (6%)	19,22,24	0.83	2 (10%)

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	C	223	2	-	0/10/11/13	0/1/1/1
2	PTR	D	248	2	-	0/10/11/13	0/1/1/1
2	PTR	C	248	2	-	1/10/11/13	0/1/1/1
2	PTR	D	223	2	-	0/10/11/13	0/1/1/1
3	PTR	E	601	3	-	2/10/11/13	0/1/1/1
4	PTR	F	601	4	-	4/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	223	PTR	OH-CZ	-4.48	1.30	1.40
2	D	223	PTR	OH-CZ	-4.39	1.30	1.40
2	D	248	PTR	OH-CZ	-4.32	1.30	1.40
4	F	601	PTR	OH-CZ	-4.06	1.31	1.40
3	E	601	PTR	OH-CZ	-3.60	1.32	1.40
3	E	601	PTR	P-OH	2.47	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	223	PTR	O2P-P-OH	2.32	112.50	105.24
4	F	601	PTR	O2P-P-OH	2.21	112.14	105.24
3	E	601	PTR	O3P-P-OH	2.21	112.14	105.24
4	F	601	PTR	O3P-P-OH	2.12	111.87	105.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	PTR	N-CA-CB-CG
4	F	601	PTR	N-CA-CB-CG
4	F	601	PTR	C-CA-CB-CG
4	F	601	PTR	CZ-OH-P-O1P
3	E	601	PTR	C-CA-CB-CG
2	C	248	PTR	CZ-OH-P-O2P
4	F	601	PTR	CZ-OH-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	PTR	1	0
4	F	601	PTR	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	502/525 (95%)	0.17	19 (3%) 44 39	57, 85, 129, 146	0
1	B	501/525 (95%)	0.31	19 (3%) 44 39	60, 90, 124, 141	0
2	C	17/37 (45%)	0.74	0 100 100	87, 116, 154, 157	0
2	D	20/37 (54%)	0.74	2 (10%) 14 12	70, 99, 126, 143	0
3	E	3/4 (75%)	1.83	1 (33%) 1 1	97, 97, 109, 111	0
4	F	3/4 (75%)	2.42	2 (66%) 0 0	134, 134, 136, 139	0
All	All	1046/1132 (92%)	0.27	43 (4%) 42 37	57, 89, 129, 157	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	CYS	3.5
1	B	236	LEU	3.5
1	A	151	VAL	3.5
1	A	125	LEU	3.2
1	A	78	VAL	3.1
1	B	318	CYS	3.0
1	A	210	LEU	3.0
1	A	245	GLN	3.0
1	B	319	ASN	3.0
1	A	236	LEU	2.9
4	F	603	ALA	2.9
2	D	221	VAL	2.8
1	B	245	GLN	2.8
1	A	126	LEU	2.8
1	B	301	VAL	2.7
1	A	132	HIS	2.7
1	A	281	ASN	2.7
2	D	228	PHE	2.7
1	A	262	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	THR	2.6
4	F	602	ALA	2.5
1	B	333	CYS	2.5
3	E	600	ALA	2.5
1	A	212	LEU	2.5
1	A	216	LEU	2.5
1	B	261	LEU	2.4
1	A	261	LEU	2.4
1	B	1	MET	2.3
1	A	319	ASN	2.3
1	B	88	LEU	2.2
1	B	381	GLY	2.2
1	B	290	VAL	2.2
1	A	135	PHE	2.2
1	B	263	TYR	2.2
1	B	341	PHE	2.2
1	A	181	VAL	2.2
1	B	262	LEU	2.1
1	A	197	TYR	2.1
1	B	367	CYS	2.1
1	B	258	GLU	2.1
1	A	170	VAL	2.1
1	B	277	ASN	2.0
1	A	152	ARG	2.0

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	C	248	16/17	0.83	0.13	108,126,130,131	0
4	PTR	F	601	16/17	0.89	0.12	90,112,134,139	0
2	PTR	D	223	16/17	0.94	0.10	76,87,91,95	0
2	PTR	D	248	16/17	0.94	0.08	77,83,87,89	0
3	PTR	E	601	16/17	0.95	0.08	63,87,105,108	0
2	PTR	C	223	16/17	0.95	0.08	69,75,83,88	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.