



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:00 AM UTC

PDB ID : 2H4V / pdb_00002h4v
Title : Crystal Structure of the Human Tyrosine Receptor Phosphatase Gamma
Authors : Ugochukwu, E.; Barr, A.; Das, S.; Eswaran, J.; Savitsky, P.; Sundstrom, M.; Edwards, A.; Arrowsmith, C.; Weigelt, J.; Debreczeni, J.; von Delft, F.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2006-05-25
Resolution : 1.55 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

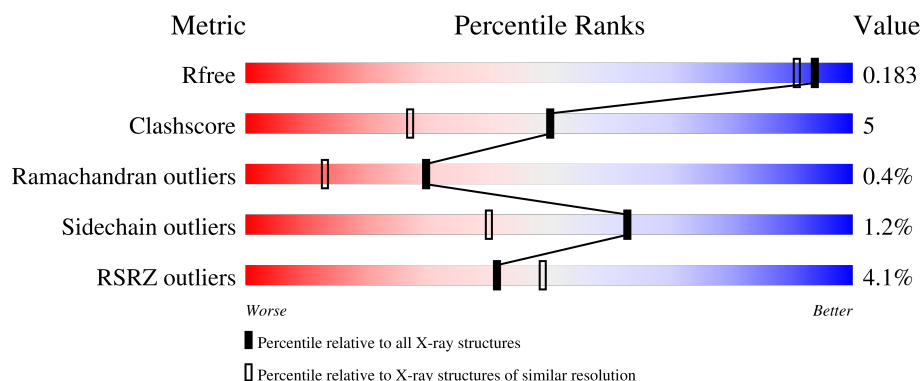
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. 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	320	
1	B	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	1129[A]	-	-	X	-
4	ACT	B	1131	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5256 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 Receptor-type tyrosine-protein phosphatase gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	15	0
			2359	1505	407	435	12			
1	B	280	Total	C	N	O	S	0	5	0
			2286	1455	403	416	12			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	808	MET	-	cloning artifact	UNP P23470
A	809	HIS	-	cloning artifact	UNP P23470
A	810	HIS	-	cloning artifact	UNP P23470
A	811	HIS	-	cloning artifact	UNP P23470
A	812	HIS	-	cloning artifact	UNP P23470
A	813	HIS	-	cloning artifact	UNP P23470
A	814	HIS	-	cloning artifact	UNP P23470
A	815	SER	-	cloning artifact	UNP P23470
A	816	SER	-	cloning artifact	UNP P23470
A	817	GLY	-	cloning artifact	UNP P23470
A	818	VAL	-	cloning artifact	UNP P23470
A	819	ASP	-	cloning artifact	UNP P23470
A	820	LEU	-	cloning artifact	UNP P23470
A	821	GLY	-	cloning artifact	UNP P23470
A	822	THR	-	cloning artifact	UNP P23470
A	823	GLU	-	cloning artifact	UNP P23470
A	824	ASN	-	cloning artifact	UNP P23470
A	825	LEU	-	cloning artifact	UNP P23470
A	826	TYR	-	cloning artifact	UNP P23470
A	827	PHE	-	cloning artifact	UNP P23470
A	828	GLN	-	cloning artifact	UNP P23470
A	829	SER	-	cloning artifact	UNP P23470
A	830	MET	-	cloning artifact	UNP P23470
B	808	MET	-	cloning artifact	UNP P23470
B	809	HIS	-	cloning artifact	UNP P23470

Continued on next page...

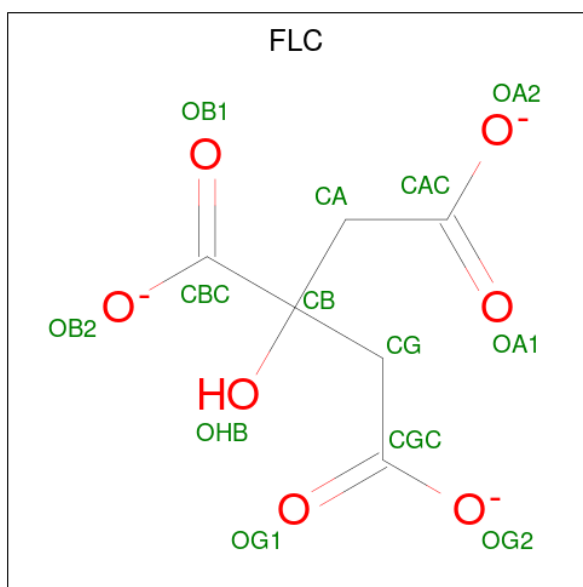
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	810	HIS	-	cloning artifact	UNP P23470
B	811	HIS	-	cloning artifact	UNP P23470
B	812	HIS	-	cloning artifact	UNP P23470
B	813	HIS	-	cloning artifact	UNP P23470
B	814	HIS	-	cloning artifact	UNP P23470
B	815	SER	-	cloning artifact	UNP P23470
B	816	SER	-	cloning artifact	UNP P23470
B	817	GLY	-	cloning artifact	UNP P23470
B	818	VAL	-	cloning artifact	UNP P23470
B	819	ASP	-	cloning artifact	UNP P23470
B	820	LEU	-	cloning artifact	UNP P23470
B	821	GLY	-	cloning artifact	UNP P23470
B	822	THR	-	cloning artifact	UNP P23470
B	823	GLU	-	cloning artifact	UNP P23470
B	824	ASN	-	cloning artifact	UNP P23470
B	825	LEU	-	cloning artifact	UNP P23470
B	826	TYR	-	cloning artifact	UNP P23470
B	827	PHE	-	cloning artifact	UNP P23470
B	828	GLN	-	cloning artifact	UNP P23470
B	829	SER	-	cloning artifact	UNP P23470
B	830	MET	-	cloning artifact	UNP P23470

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

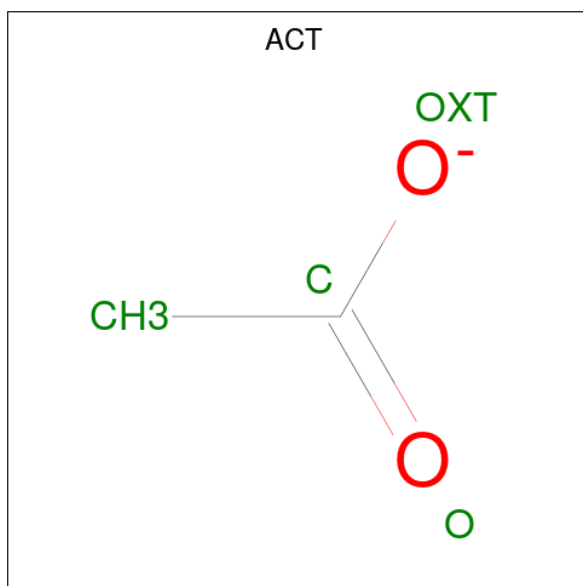
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cl 4 4	0	0
2	B	3	Total Cl 3 3	0	0

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

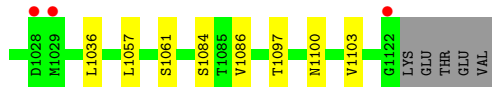
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	281	Total O 283 283	0	2
7	B	278	Total O 279 279	0	1

i

- Molecule 1: Receptor-type tyrosine-protein phosphatase gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.85Å 78.86Å 121.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 1.55 47.23 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.23-1.55) 100.0 (47.23-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.161 , 0.181 0.168 , 0.183	Depositor DCC
R_{free} test set	5245 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5256	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.333 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: FLC, EDO, ACT, CL, NA

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	0.74	0/2441	0.81	0/3307
1	B	0.71	0/2353	0.82	3/3186 (0.1%)
All	All	0.73	0/4794	0.82	3/6493 (0.0%)

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	A	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1036	LEU	CA-C-N	-5.49	113.24	119.28
1	B	1036	LEU	C-N-CA	-5.49	113.24	119.28
1	B	914	GLY	N-CA-C	-5.39	105.19	112.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	916[A]	ASN	CA

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	2359	0	2309	32	0
1	B	2286	0	2241	12	0
2	A	4	0	0	2	0
2	B	3	0	0	1	0
3	A	13	0	5	1	0
4	A	4	0	3	5	0
4	B	4	0	3	2	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
6	B	1	0	0	0	0
7	A	283	0	0	6	0
7	B	279	0	0	1	0
All	All	5256	0	4591	49	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 (49) 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:915[A]:TYR:OH	1:A:1083[A]:LYS:CD	1.88	1.21
1:B:862[A]:MET:HE1	1:B:1097:THR:CG2	1.97	0.94
1:A:988[B]:CYS:SG	7:A:274:HOH:O	2.29	0.90
1:A:841:TYR:OH	1:A:1114[B]:ASP:OD1	1.92	0.87
1:B:862[A]:MET:HE1	1:B:1097:THR:HG22	1.57	0.85
1:A:939[A]:ILE:HD11	1:A:1057:LEU:HD13	1.60	0.83
4:A:1129[A]:ACT:OXT	4:B:1131:ACT:H3	1.78	0.82
1:A:988[B]:CYS:HA	1:A:1025:GLN:HG2	1.69	0.74
1:A:988[A]:CYS:HA	1:A:1025:GLN:HG2	1.70	0.74
1:A:1083[A]:LYS:O	1:A:1084[A]:SER:HB2	1.88	0.73
1:A:826:TYR:N	1:A:1084[B]:SER:HB3	2.06	0.71
1:B:1061[B]:SER:OG	7:B:657:HOH:O	1.98	0.71
1:A:829:SER:OG	1:A:1084[B]:SER:O	2.11	0.68
1:A:970:SER:HB3	1:A:977[A]:ILE:HD11	1.75	0.68
1:B:862[A]:MET:CE	1:B:1097:THR:HG22	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ILE:HD11	1:B:862[B]:MET:HE3	1.82	0.62
1:B:833:PHE:CG	1:B:1086:VAL:HG11	2.35	0.62
1:B:856[B]:GLN:NE2	2:B:1129:CL:CL	2.70	0.61
1:A:826:TYR:N	1:A:1084[A]:SER:HG	1.98	0.61
1:A:1079:GLN:NE2	1:A:1085[A]:THR:O	2.34	0.61
4:A:1129[A]:ACT:H2	7:A:616:HOH:O	2.02	0.59
1:A:1114[B]:ASP:OD2	7:A:418:HOH:O	2.17	0.59
1:A:830:MET:HA	1:A:830:MET:HE2	1.89	0.54
1:A:1084[A]:SER:O	1:A:1085[A]:THR:O	2.26	0.54
1:A:971:GLU:O	1:A:977[A]:ILE:HD12	2.08	0.53
1:A:1083[B]:LYS:CD	1:A:1085[B]:THR:OG1	2.55	0.53
1:A:1074:ASP:OD2	2:A:801:CL:CL	2.64	0.53
4:A:1129[A]:ACT:C	7:A:616:HOH:O	2.57	0.52
1:B:862[A]:MET:HE1	1:B:1097:THR:CB	2.40	0.52
1:A:833:PHE:CG	1:A:1086:VAL:HG11	2.46	0.51
1:A:1084[A]:SER:O	1:A:1085[A]:THR:C	2.55	0.50
3:A:1128:FLC:HA1	7:A:362:HOH:O	2.12	0.49
1:A:915[A]:TYR:HH	1:A:1083[A]:LYS:CD	2.20	0.49
1:A:1083[A]:LYS:O	1:A:1084[A]:SER:CB	2.61	0.48
1:A:1057:LEU:C	1:A:1057:LEU:HD23	2.42	0.45
1:B:830:MET:HE3	1:B:1084:SER:C	2.42	0.45
1:A:977[A]:ILE:CG2	1:A:997:ARG:HB3	2.47	0.45
1:A:988[B]:CYS:HA	1:A:1025:GLN:CG	2.43	0.44
4:A:1129[A]:ACT:H1	4:B:1131:ACT:CH3	2.48	0.43
1:A:988[A]:CYS:HA	1:A:1025:GLN:CG	2.44	0.43
1:A:826:TYR:N	1:A:1084[B]:SER:CB	2.79	0.43
1:B:830:MET:HA	1:B:830:MET:HE2	2.00	0.42
1:B:1057:LEU:C	1:B:1057:LEU:HD23	2.45	0.42
1:A:907:ILE:HG13	2:A:805:CL:CL	2.57	0.42
1:A:1046[B]:SER:OG	1:A:1078[B]:GLN:NE2	2.53	0.42
1:B:862[A]:MET:HE1	1:B:1097:THR:HB	2.01	0.42
1:A:915[A]:TYR:CE1	1:A:1079:GLN:HG3	2.55	0.41
4:A:1129[A]:ACT:CH3	7:A:616:HOH:O	2.66	0.41
1:A:971:GLU:C	1:A:977[A]:ILE:HD12	2.46	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	287/320 (90%)	270 (94%)	16 (6%)	1 (0%)	36	18
1	B	279/320 (87%)	269 (96%)	9 (3%)	1 (0%)	30	13
All	All	566/640 (88%)	539 (95%)	25 (4%)	2 (0%)	30	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1103	VAL
1	B	1103	VAL

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	259/286 (91%)	255 (98%)	4 (2%)	57	31
1	B	248/286 (87%)	245 (99%)	3 (1%)	63	40
All	All	507/572 (89%)	500 (99%)	7 (1%)	63	33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	916[A]	ASN
1	A	916[B]	ASN
1	A	1081	LYS
1	A	1100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	901	SER
1	B	956	LYS
1	B	1100	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	846	HIS
1	A	870	ASN
1	A	952	ASN
1	A	975	ASN
1	B	846	HIS
1	B	963	GLN
1	B	1079	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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
5	EDO	A	703	-	3,3,3	0.38	0	2,2,2	0.36	0
5	EDO	B	701	-	3,3,3	0.44	0	2,2,2	0.09	0
4	ACT	B	1131	-	3,3,3	1.06	0	3,3,3	1.06	0
3	FLC	A	1128	-	12,12,12	1.16	0	17,17,17	1.29	2 (11%)
5	EDO	B	705	-	3,3,3	0.39	0	2,2,2	0.52	0
5	EDO	A	702	-	3,3,3	0.49	0	2,2,2	0.27	0
4	ACT	A	1129[A]	-	3,3,3	0.91	0	3,3,3	1.24	0
5	EDO	A	704	-	3,3,3	0.31	0	2,2,2	0.30	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
5	EDO	A	703	-	-	0/1/1/1	-
5	EDO	B	701	-	-	0/1/1/1	-
3	FLC	A	1128	-	-	3/16/16/16	-
5	EDO	B	705	-	-	0/1/1/1	-
5	EDO	A	702	-	-	0/1/1/1	-
5	EDO	A	704	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1128	FLC	OB2-CBC-CB	2.79	118.50	113.14
3	A	1128	FLC	OG1-CGC-CG	-2.18	116.78	122.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1128	FLC	CBC-CB-CG-CGC
3	A	1128	FLC	OHB-CB-CG-CGC
3	A	1128	FLC	CA-CB-CG-CGC

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1131	ACT	2	0
3	A	1128	FLC	1	0
4	A	1129[A]	ACT	5	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, 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	278/320 (86%)	0.08	12 (4%)	40 48	7, 16, 32, 54	15 (5%)
1	B	280/320 (87%)	0.11	11 (3%)	43 51	10, 18, 33, 49	5 (1%)
All	All	558/640 (87%)	0.10	23 (4%)	41 49	7, 17, 33, 54	20 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	826	TYR	6.8
1	B	1001	VAL	6.4
1	A	915[A]	TYR	6.3
1	A	1085[A]	THR	6.2
1	A	897	PRO	4.1
1	B	915	TYR	3.6
1	B	897	PRO	3.4
1	A	1084[A]	SER	3.4
1	A	916[A]	ASN	3.1
1	A	1083[A]	LYS	3.0
1	B	1014	ASN	3.0
1	A	827	PHE	2.9
1	B	1122	GLY	2.9
1	A	896	LEU	2.8
1	A	1082	ASP	2.7
1	B	1000	LYS	2.4
1	B	916	ASN	2.4
1	A	843	ASN	2.2
1	B	858	CYS	2.2
1	A	1122	GLY	2.2
1	B	1028	ASP	2.2
1	B	1029	MET	2.1
1	B	859	THR	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	CL	A	806	1/1	0.75	0.25	71,71,71,71	0
4	ACT	B	1131	4/4	0.78	0.17	27,34,36,42	0
2	CL	A	803	1/1	0.79	0.25	55,55,55,55	0
4	ACT	A	1129[A]	4/4	0.81	0.23	12,22,22,22	4
3	FLC	A	1128	13/13	0.82	0.16	26,54,63,66	0
2	CL	B	804	1/1	0.86	0.16	60,60,60,60	0
5	EDO	B	705	4/4	0.87	0.14	24,31,38,42	0
2	CL	B	1129	1/1	0.90	0.26	51,51,51,51	0
2	CL	B	1128	1/1	0.91	0.13	62,62,62,62	0
5	EDO	B	701	4/4	0.92	0.13	23,25,25,26	0
5	EDO	A	704	4/4	0.96	0.16	20,27,30,31	0
5	EDO	A	702	4/4	0.96	0.13	14,20,24,27	0
5	EDO	A	703	4/4	0.96	0.12	17,21,26,27	0
2	CL	A	801	1/1	0.98	0.22	34,34,34,34	0
6	NA	B	1130	1/1	0.98	0.13	24,24,24,24	0
2	CL	A	805	1/1	0.99	0.19	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.