Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 05:28 AM EST

PDB ID	:	4NWF
Title	:	Crystal structure of the tyrosine phosphatase SHP-2 with N308D mutation
Authors	:	Qiu, W.; Lin, A.; Hutchinson, A.; Romanov, V.; Ruzanov, M.; Thompson, C.; Lam, K.; Kisselman, G.; Battalie, K.; Chirgadze, N.Y.
Deposited on	:	2013-12-06
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36
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)	:	2.36

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 2.10 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.
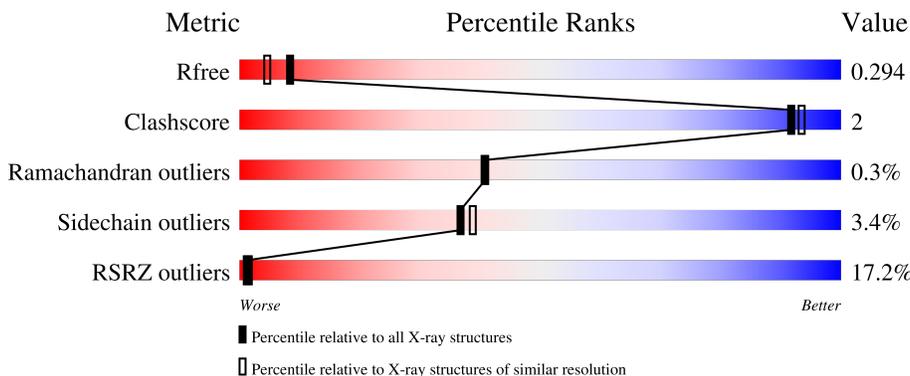
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	539	16% / 82% / 8% / 9%
1	B	539	15% / 86% / 6% / 8%

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
2	EDO	A	605	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8689 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	A	489	Total	C	N	O	S	0	1	0
			3975	2501	708	748	18			
1	B	496	Total	C	N	O	S	0	2	0
			4025	2529	716	761	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ASP	ASN	engineered mutation	UNP Q06124
A	?	-	GLN	deletion	UNP Q06124
A	?	-	ALA	deletion	UNP Q06124
A	?	-	LEU	deletion	UNP Q06124
A	?	-	LEU	deletion	UNP Q06124
B	308	ASP	ASN	engineered mutation	UNP Q06124
B	?	-	GLN	deletion	UNP Q06124
B	?	-	ALA	deletion	UNP Q06124
B	?	-	LEU	deletion	UNP Q06124
B	?	-	LEU	deletion	UNP Q06124

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
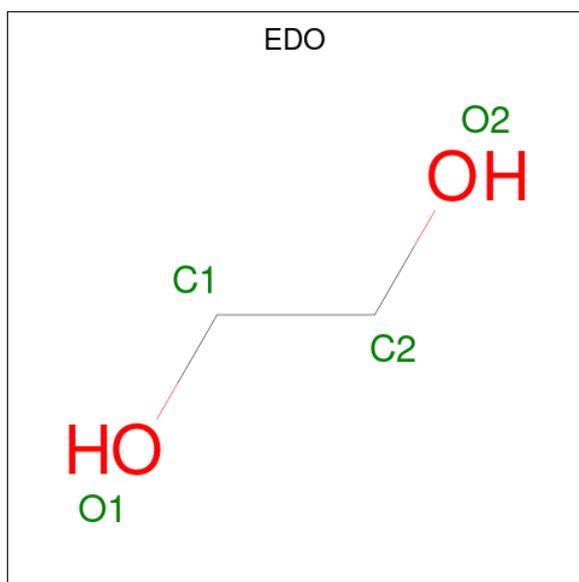
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

W O R L D W I D E

PDB

PROTEIN DATA BANK

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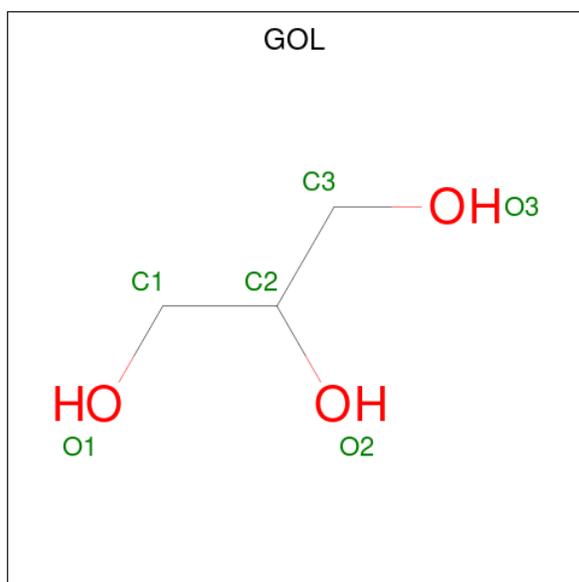
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	326	Total 326	O 326	0	0
4	B	329	Total 329	O 329	0	0

3 Residue-property plots ⓘ

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 A:

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

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.28Å 55.88Å 91.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 100.0 (19.98-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.09Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.266 , 0.309 0.260 , 0.294	Depositor DCC
R_{free} test set	954 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.9	EDS
L-test for twinning[2]	$< |L| > = 0.56, < L^2 > = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 65.68 % 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 6.8214e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: GOL, EDO

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	0/4058	0.56	0/5471
1	B	0.38	0/4107	0.56	0/5536
All	All	0.38	0/8165	0.56	0/11007

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	3975	0	3895	15	0
1	B	4025	0	3944	12	0
2	A	16	0	24	0	0
2	B	12	0	18	0	0
3	A	6	0	8	0	0
4	A	326	0	0	0	0
4	B	329	0	0	0	0
All	All	8689	0	7889	25	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 2.

All (25) 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:432:PRO:HG3	1:A:516:MET:HG2	1.89	0.55
1:B:432:PRO:HG3	1:B:516:MET:HG2	1.90	0.53
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.90	0.53
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.90	0.53
1:A:149:LEU:HB2	1:A:172:ILE:HD11	1.97	0.47
1:A:25:VAL:HG11	1:B:175:GLN:HB3	1.97	0.46
1:A:526:GLN:HA	1:A:529:ILE:HD12	1.98	0.45
1:B:55:LYS:HE3	1:B:57:GLN:HB3	1.99	0.45
1:B:149:LEU:HB2	1:B:172:ILE:HD11	1.98	0.45
1:A:88:LEU:HD23	1:A:96:ILE:HB	1.98	0.44
1:A:175:GLN:HB3	1:B:25:VAL:HG11	1.99	0.44
1:A:377:LEU:HD13	1:A:386:ARG:HB2	2.00	0.44
1:A:117:LEU:HD22	1:A:121:GLU:HB3	1.99	0.44
1:A:310:ILE:HB	1:A:327:TYR:HB2	2.00	0.43
1:B:310:ILE:HB	1:B:327:TYR:HB2	2.01	0.43
1:B:377:LEU:HD13	1:B:386:ARG:HB2	2.00	0.43
1:A:11:ILE:HD11	1:A:19:LEU:HD12	2.01	0.43
1:B:125:LEU:HB3	1:B:216:LEU:HD21	2.01	0.43
1:A:139:GLU:HG2	1:A:147:PHE:CE2	2.54	0.43
1:B:227:GLU:HG3	1:B:519:GLN:HE21	1.84	0.42
1:A:125:LEU:HB3	1:A:216:LEU:HD21	2.01	0.42
1:A:115:GLY:HA2	1:A:139:GLU:HG3	2.02	0.41
1:B:54:ILE:HG12	1:B:89:LYS:HD3	2.03	0.41
1:B:290:VAL:HG11	1:B:344:MET:HG3	2.04	0.40
1:A:227:GLU:HG3	1:A:519:GLN:HE21	1.85	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	476/539 (88%)	467 (98%)	7 (2%)	2 (0%)	34	32
1	B	484/539 (90%)	475 (98%)	8 (2%)	1 (0%)	47	49
All	All	960/1078 (89%)	942 (98%)	15 (2%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	A	505	VAL
1	B	505	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	436/480 (91%)	418 (96%)	18 (4%)	30	31
1	B	442/480 (92%)	430 (97%)	12 (3%)	44	48
All	All	878/960 (92%)	848 (97%)	30 (3%)	37	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	55	LYS
1	A	90	GLU
1	A	96	ILE
1	A	98	LEU
1	A	171	MET
1	A	177	LEU
1	A	199	LYS
1	A	205	THR
1	A	226	ILE
1	A	326	SER
1	A	408	GLN
1	A	413	ARG

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Mol	Chain	Res	Type
1	A	477	ASP
1	A	502	SER
1	A	527	ARG
1	A	528	ARG
1	A	533	GLN
1	B	47	ARG
1	B	87	GLN
1	B	98	LEU
1	B	155	ASP
1	B	177	LEU
1	B	199	LYS
1	B	226	ILE
1	B	294	ASP
1	B	326	SER
1	B	413	ARG
1	B	502	SER
1	B	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	141	GLN
1	A	519	GLN
1	B	298	ASN
1	B	519	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	EDO	B	601	-	3,3,3	0.57	0	2,2,2	0.27	0
2	EDO	A	605	-	3,3,3	0.54	0	2,2,2	0.21	0
2	EDO	A	604	-	3,3,3	0.61	0	2,2,2	0.24	0
3	GOL	A	602	-	5,5,5	0.07	0	5,5,5	0.15	0
2	EDO	A	601	-	3,3,3	0.58	0	2,2,2	0.32	0
2	EDO	B	603	-	3,3,3	0.57	0	2,2,2	0.32	0
2	EDO	B	602	-	3,3,3	0.61	0	2,2,2	0.21	0
2	EDO	A	603	-	3,3,3	0.54	0	2,2,2	0.27	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	EDO	B	601	-	-	0/1/1/1	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
3	GOL	A	602	-	-	0/4/4/4	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-

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.

No monomer is involved in short contacts.

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	489/539 (90%)	1.03	87 (17%)	1	1	16, 37, 65, 106	0
1	B	496/539 (92%)	1.03	82 (16%)	1	2	17, 37, 67, 100	0
All	All	985/1078 (91%)	1.03	169 (17%)	1	1	16, 37, 66, 106	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	HIS	10.2
1	A	409	GLY	7.7
1	A	177	LEU	7.0
1	B	141	GLN	6.7
1	B	155	ASP	6.4
1	B	37	ASN	6.2
1	B	177	LEU	6.1
1	A	154	GLY	6.1
1	B	298	ASN	6.0
1	A	3	SER	5.4
1	A	207	GLY	5.4
1	B	38	PRO	5.4
1	B	164	LYS	5.3
1	B	36	SER	5.3
1	B	86	GLY	5.2
1	A	66	TYR	5.1
1	A	141	GLN	5.1
1	A	144	PRO	5.0
1	A	89	LYS	5.0
1	A	165	SER	5.0
1	B	144	PRO	4.9
1	A	85[A]	HIS	4.9
1	B	205	THR	4.7
1	B	143	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	SER	4.4
1	B	48	ASN	4.3
1	B	451	ASP	4.3
1	A	224	ALA	4.2
1	A	48	ASN	4.1
1	A	149	LEU	4.1
1	A	116	HIS	4.0
1	B	142	SER	4.0
1	A	296	ASP	4.0
1	B	165	SER	4.0
1	A	248	TRP	3.9
1	B	96	ILE	3.9
1	B	207	GLY	3.8
1	B	14	VAL	3.8
1	B	68	GLY	3.8
1	A	143	HIS	3.8
1	A	525	LEU	3.8
1	A	527	ARG	3.8
1	A	262	LEU	3.8
1	A	522	ILE	3.7
1	A	450	MET	3.7
1	B	3	SER	3.6
1	A	206	LEU	3.6
1	B	231	ARG	3.5
1	B	163	GLY	3.5
1	B	294	ASP	3.4
1	A	297	PRO	3.4
1	B	206	LEU	3.4
1	B	296	ASP	3.4
1	A	226	ILE	3.4
1	B	248	TRP	3.4
1	A	514	ILE	3.3
1	B	529	ILE	3.3
1	A	203	VAL	3.3
1	A	148	VAL	3.2
1	B	120	LYS	3.1
1	B	156	ASP	3.1
1	A	125	LEU	3.1
1	B	196	HIS	3.1
1	A	231	ARG	3.1
1	A	223	ALA	3.1
1	B	88	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	451	ASP	3.1
1	B	127	THR	3.1
1	B	35	LYS	3.1
1	B	282	ILE	3.0
1	B	409	GLY	3.0
1	B	47	ARG	3.0
1	B	212	LEU	3.0
1	A	394	HIS	3.0
1	A	205	THR	2.9
1	A	294	ASP	2.9
1	A	127	THR	2.9
1	B	362	ARG	2.9
1	A	117	LEU	2.9
1	B	262	LEU	2.9
1	B	209	VAL	2.9
1	A	529	ILE	2.9
1	B	353	ILE	2.9
1	B	224	ALA	2.8
1	A	532	GLU	2.8
1	A	10	ASN	2.8
1	A	151	VAL	2.8
1	B	527	ARG	2.8
1	A	108	THR	2.7
1	A	488	ILE	2.7
1	A	528	ARG	2.7
1	A	218	THR	2.7
1	B	305	ILE	2.7
1	A	228	SER	2.7
1	B	228	SER	2.7
1	B	475	LEU	2.7
1	A	518	VAL	2.6
1	B	204	GLU	2.6
1	A	86	GLY	2.6
1	B	295	GLY	2.6
1	B	313	GLU	2.6
1	B	151	VAL	2.6
1	B	87	GLN	2.6
1	B	301	VAL	2.6
1	B	118	SER	2.6
1	B	62	TYR	2.5
1	B	66	TYR	2.5
1	A	293	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	263	TYR	2.5
1	A	155	ASP	2.5
1	A	225	GLU	2.5
1	A	172	ILE	2.5
1	B	234	SER	2.5
1	B	154	GLY	2.5
1	A	533	GLN	2.5
1	A	171	MET	2.4
1	A	233	LEU	2.4
1	A	230	VAL	2.4
1	B	211	GLN	2.4
1	A	284	PRO	2.4
1	B	450	MET	2.4
1	B	149	LEU	2.4
1	A	301	VAL	2.4
1	A	311	MET	2.4
1	A	261	LEU	2.4
1	A	295	GLY	2.4
1	A	169	HIS	2.3
1	A	520	HIS	2.3
1	B	128	GLU	2.3
1	A	490	VAL	2.3
1	A	147	PHE	2.3
1	B	23	ARG	2.3
1	B	171	MET	2.3
1	B	311	MET	2.3
1	A	74	LEU	2.2
1	B	194	VAL	2.2
1	A	437	ASP	2.2
1	B	223	ALA	2.2
1	B	218	THR	2.2
1	B	525	LEU	2.2
1	A	90	GLU	2.2
1	B	22	THR	2.2
1	A	439	LEU	2.2
1	B	272	GLU	2.2
1	B	297	PRO	2.2
1	A	479	ILE	2.1
1	B	95	VAL	2.1
1	A	14	VAL	2.1
1	A	95	VAL	2.1
1	B	485	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLY	2.1
1	A	456	VAL	2.1
1	B	203	VAL	2.1
1	A	259	CYS	2.1
1	A	23	ARG	2.1
1	A	530	GLU	2.1
1	A	11	ILE	2.1
1	A	126	LEU	2.1
1	B	261	LEU	2.1
1	B	392	ALA	2.1
1	A	87	GLN	2.1
1	B	166	LYS	2.1
1	A	210	LEU	2.0
1	B	514	ILE	2.0
1	B	415	VAL	2.0
1	A	266	LYS	2.0
1	B	117	LEU	2.0
1	A	485	ASP	2.0
1	A	256	GLN	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	GOL	A	602	6/6	0.52	0.28	52,53,53,53	0
2	EDO	B	602	4/4	0.60	0.32	51,51,51,52	0
2	EDO	A	601	4/4	0.62	0.27	55,55,55,55	0
2	EDO	B	601	4/4	0.70	0.29	52,52,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	603	4/4	0.72	0.37	61,62,62,63	0
2	EDO	A	605	4/4	0.75	0.41	46,46,46,48	0
2	EDO	B	603	4/4	0.78	0.23	54,54,55,55	0
2	EDO	A	604	4/4	0.83	0.27	38,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.