



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:18 PM GMT

PDB ID : 2V4M
Title : THE ISOMERASE DOMAIN OF HUMAN GLUTAMINE-FRUCTOSE-6-PHOSPHATETRANSAMINASE 1 (GFPT1) IN COMPLEX WITH FRUCTOSE 6-PHOSPHATE
Authors : Moche, M.; Lehtio, L.; Andersson, J.; Arrowsmith, C.H.; Berglund, H.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Nilsson, M.E.; Nyman, T.; Persson, C.; Sagemark, J.; Svensson, S.; Schueler, H.; Thorsell, A.G.; Tresaugues, L.; Uppenberg, J.; Van Den Berg, S.; Welin, M.; Wisniewska, M.; Weigelt, J.; Nordlund, P.; Wikstrom, M.
Deposited on : 2008-09-26
Resolution : 2.29 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

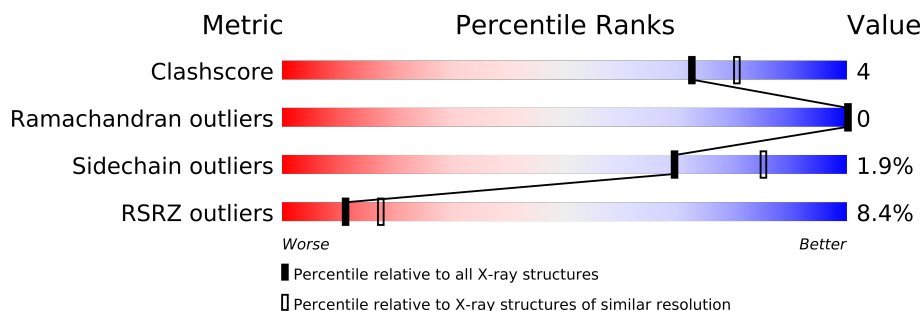
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.29 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	

2 Entry composition i

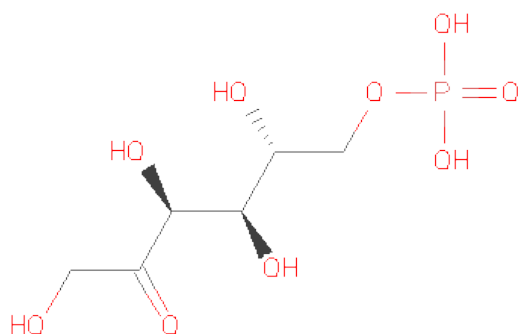
There are 4 unique types of molecules in this entry. The entry contains 11333 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLUCOSAMINE--FRUCTOSE-6-PHOSPHATEAMINO-TRANSFERASE [ISOMERIZING] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	3	0
			2775	1747	482	518	28			
1	B	351	Total	C	N	O	S	0	2	0
			2762	1739	481	516	26			
1	C	352	Total	C	N	O	S	0	4	0
			2794	1760	488	519	27			
1	D	350	Total	C	N	O	S	0	4	0
			2773	1745	483	518	27			

- Molecule 2 is FRUCTOSE -6-PHOSPHATE (three-letter code: F6R) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

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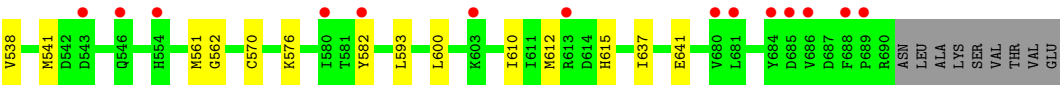
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		

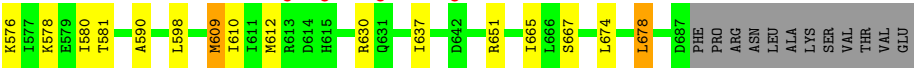
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	14	Total	O	0	0
			14	14		
4	C	50	Total	O	0	0
			50	50		
4	D	65	Total	O	0	0
			65	65		



● Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATEAMINOTRANSFERASE [ISOMERIZING] 1

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	178.82Å 178.82Å 157.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.89 – 2.29 54.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.89-2.29) 96.8 (54.85-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.167 , 0.185 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.6	EDS
Estimated twinning fraction	0.679 for H, K, L 0.321 for -H-K, K, -L 0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.679 for H, K, L 0.321 for -H-K, K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 81887 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11333	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6R, CL

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	0.41	0/2815	0.56	0/3794
1	B	0.37	0/2803	0.52	0/3780
1	C	0.45	0/2836	0.59	0/3824
1	D	0.47	0/2813	0.60	0/3792
All	All	0.43	0/11267	0.57	0/15190

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	0	2833	19	0
1	B	2762	0	2814	41	0
1	C	2794	0	2849	19	0
1	D	2773	0	2829	20	0
2	A	16	0	11	0	0
2	B	16	0	11	1	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	35	0	0	0	0
4	B	14	0	0	0	0
4	C	50	0	0	0	0
4	D	65	0	0	0	0
All	All	11333	0	11369	97	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:563:ARG:HG3	1:D:590:ALA:HB3	1.40	1.01
1:B:548:LEU:HD22	1:B:653:ILE:HD11	1.63	0.81
1:D:612:MET:CE	1:D:637:ILE:HG22	2.17	0.74
1:D:491:ALA:HB1	1:D:576:LYS:HE3	1.71	0.73
1:C:508:LEU:O	1:C:521[A]:ARG:NH1	2.23	0.71
1:D:612:MET:HE1	1:D:637:ILE:HG22	1.72	0.70
1:B:576:LYS:NZ	2:B:800:F6R:O1	2.23	0.67
1:B:550:THR:HG22	1:B:681:LEU:HD21	1.76	0.67
1:A:570[B]:CYS:SG	1:A:610:ILE:HD12	2.38	0.63
1:B:389:LEU:HD12	1:B:416:VAL:HG22	1.81	0.62
1:D:362:VAL:HG13	1:D:525:MET:HE3	1.82	0.61
1:D:570[B]:CYS:SG	1:D:610:ILE:HD12	2.42	0.60
1:B:396:TYR:CE1	1:B:416:VAL:HG12	2.37	0.60
1:A:611:ILE:HD12	1:A:620:CYS:HB3	1.85	0.59
1:B:384:CYS:SG	1:B:434:VAL:HG23	2.43	0.59
1:B:417:GLU:OE1	1:B:425:ARG:NH2	2.35	0.58
1:B:569:THR:HG21	1:B:610:ILE:HD13	1.85	0.58
1:B:343:MET:CE	1:B:347:ILE:HD11	2.36	0.55
1:D:343:MET:SD	1:D:580:ILE:HD13	2.47	0.54
1:B:548:LEU:HD21	1:B:635:VAL:HG11	1.89	0.54
1:C:491:ALA:HB1	1:C:576:LYS:HE3	1.90	0.54
1:B:573:GLY:HA3	1:B:671:LEU:HD13	1.91	0.53
1:B:655:VAL:HG13	1:B:656:PRO:HD2	1.91	0.52
1:C:362:VAL:HG13	1:C:525:MET:CE	2.40	0.52
1:B:659:VAL:HG12	1:B:662:LEU:HD12	1.91	0.52
1:D:598:LEU:O	1:D:630:ARG:NH1	2.42	0.52
1:B:569:THR:CG2	1:B:610:ILE:HD13	2.39	0.52
1:D:354:VAL:HG12	1:D:358:MET:HE2	1.91	0.52
1:B:611:ILE:HD12	1:B:636:VAL:HG13	1.92	0.52
1:A:612:MET:HE2	1:A:637:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:570[B]:CYS:SG	1:C:610:ILE:HD12	2.51	0.51
1:A:531:LEU:HD21	1:A:665:ILE:HD13	1.93	0.51
1:B:442:GLY:HA2	1:B:472:ILE:HD12	1.93	0.51
1:B:388:ILE:HD13	1:B:415:MET:HE2	1.92	0.51
1:A:437:PHE:CZ	1:A:451:LEU:HA	2.46	0.50
1:B:343:MET:HE2	1:B:347:ILE:HD11	1.93	0.50
1:C:561:MET:SD	1:C:593:LEU:HD11	2.51	0.50
1:C:362:VAL:HG11	1:C:364:PHE:CE1	2.47	0.50
1:B:635:VAL:HG22	1:B:651:ARG:HD2	1.94	0.50
1:A:361:ARG:HG2	1:A:371:LEU:HD23	1.93	0.49
1:A:583:MET:CE	1:A:678:LEU:HD21	2.43	0.49
1:A:560:ILE:HD11	1:A:577:ILE:HD12	1.95	0.49
1:C:437:PHE:CZ	1:C:451:LEU:HA	2.49	0.48
1:C:356:ASN:OD1	1:C:359:ARG:NH1	2.46	0.48
1:B:567:TYR:CD1	1:B:589:LEU:HD13	2.49	0.48
1:D:569:THR:HG21	1:D:667[A]:SER:OG	2.14	0.48
1:B:611:ILE:HD12	1:B:636:VAL:CG1	2.44	0.48
1:C:439:SER:O	1:C:465:THR:HA	2.14	0.48
1:B:577:ILE:CG2	1:B:583:MET:HE3	2.43	0.47
1:D:437:PHE:CZ	1:D:451:LEU:HA	2.48	0.47
1:D:531:LEU:HD21	1:D:665:ILE:HD13	1.95	0.47
1:B:562:GLY:HA3	1:B:570[B]:CYS:SG	2.54	0.47
1:A:610:ILE:O	1:A:611:ILE:HD13	2.15	0.47
1:C:612:MET:CE	1:C:637:ILE:HG22	2.44	0.47
1:D:674:LEU:HG	1:D:678:LEU:HD22	1.97	0.46
1:A:535:ILE:HG23	1:A:669:ILE:CD1	2.45	0.46
1:B:379:LYS:HA	1:B:382:GLN:HE21	1.81	0.46
1:D:354:VAL:CG1	1:D:358:MET:HE2	2.45	0.46
1:B:550:THR:CG2	1:B:681:LEU:HD11	2.46	0.46
1:B:508:LEU:HD22	1:B:521:ARG:HB2	1.97	0.45
1:B:550:THR:HG22	1:B:681:LEU:HD11	1.99	0.45
1:B:534:LEU:HD22	1:B:656:PRO:HB2	1.99	0.45
1:B:351:PRO:HG3	1:B:535:ILE:HG22	1.99	0.45
1:B:347:ILE:HG21	1:B:673:LEU:CD2	2.47	0.44
1:B:437:PHE:CZ	1:B:451:LEU:HA	2.51	0.44
1:A:674:LEU:O	1:A:678:LEU:HB2	2.17	0.44
1:B:500:PHE:O	1:B:504:VAL:HG23	2.17	0.44
1:A:491:ALA:HB1	1:A:576:LYS:HE3	1.99	0.44
1:A:439:SER:O	1:A:465:THR:HA	2.18	0.43
1:B:577:ILE:HG21	1:B:583:MET:HE3	1.99	0.43
1:A:535:ILE:HG23	1:A:669:ILE:HD13	2.00	0.43
1:D:492:SER:OG	1:D:495:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:MET:SD	1:A:580:ILE:HD13	2.59	0.43
1:A:380:GLU:HG2	1:C:431:ARG:HD2	2.00	0.43
1:D:354:VAL:HG12	1:D:358:MET:CE	2.48	0.42
1:B:548:LEU:CD2	1:B:653:ILE:HD11	2.43	0.42
1:C:562:GLY:N	1:C:570[B]:CYS:SG	2.92	0.42
1:D:350:GLN:HA	1:D:353:SER:OG	2.19	0.42
1:B:636:VAL:HG23	1:B:649:THR:HG21	2.02	0.42
1:A:612:MET:CE	1:A:637:ILE:HG22	2.50	0.42
1:C:612:MET:HE1	1:C:637:ILE:HG22	2.02	0.42
1:D:609:MET:HE2	1:D:609:MET:HB2	1.98	0.42
1:A:347:ILE:HG13	1:A:493:THR:HG21	2.02	0.42
1:B:384:CYS:SG	1:B:434:VAL:CG2	3.07	0.41
1:C:402:THR:HG21	1:C:503:LEU:HB2	2.03	0.41
1:C:362:VAL:HG13	1:C:525:MET:HE1	2.02	0.41
1:B:560:ILE:HG22	1:B:570[B]:CYS:SG	2.61	0.41
1:C:384[A]:CYS:CB	1:C:434:VAL:HG23	2.50	0.41
1:C:492:SER:O	1:C:576:LYS:HE2	2.21	0.41
1:B:569:THR:CG2	1:B:610:ILE:CD1	2.99	0.40
1:A:531:LEU:HD21	1:A:665:ILE:CD1	2.51	0.40
1:B:676:PHE:CD1	1:B:686:VAL:HG21	2.56	0.40
1:D:423:LEU:HD11	1:D:449[B]:MET:HB2	2.04	0.40
1:C:538:VAL:O	1:C:541:MET:HG2	2.21	0.40
1:B:669:ILE:HB	1:B:670:PRO:HD3	2.04	0.40
1:B:367:TYR:HD2	1:B:525:MET:HE3	1.86	0.40
1:C:600:LEU:HD22	1:D:578:LYS:HG2	2.04	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	353/376 (94%)	342 (97%)	11 (3%)	0	100	100
1	B	351/376 (93%)	344 (98%)	7 (2%)	0	100	100
1	C	354/376 (94%)	349 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100	100
All	All	1410/1504 (94%)	1381 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/330 (94%)	309 (99%)	2 (1%)	92	97
1	B	309/330 (94%)	302 (98%)	7 (2%)	63	80
1	C	313/330 (95%)	306 (98%)	7 (2%)	64	81
1	D	311/330 (94%)	304 (98%)	7 (2%)	63	80
All	All	1244/1320 (94%)	1221 (98%)	23 (2%)	69	86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	PHE
1	A	622	ASN
1	B	385	ARG
1	B	440	GLN
1	B	457	ARG
1	B	581	THR
1	B	594	LYS
1	B	612	MET
1	B	654	LYS
1	C	440	GLN
1	C	457	ARG
1	C	500	PHE
1	C	525	MET
1	C	582	TYR
1	C	615	HIS
1	C	641	GLU
1	D	352	GLU

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Mol	Chain	Res	Type
1	D	471	SER
1	D	500	PHE
1	D	581	THR
1	D	609	MET
1	D	651	ARG
1	D	678	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	ASN
1	B	382	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
2	F6R	A	800	-	15,15,15	0.67	0	21,21,21	1.21	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	F6R	B	800	-	15,15,15	0.56	0	21,21,21	0.93	1 (4%)
2	F6R	C	800	-	15,15,15	0.62	0	21,21,21	1.19	2 (9%)
2	F6R	D	800	-	15,15,15	0.77	0	21,21,21	1.06	1 (4%)

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	F6R	A	800	-	-	0/20/20/20	0/0/0/0
2	F6R	B	800	-	-	0/20/20/20	0/0/0/0
2	F6R	C	800	-	-	0/20/20/20	0/0/0/0
2	F6R	D	800	-	-	0/20/20/20	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	F6R	C4-C3-C2	2.89	114.50	110.77
2	A	800	F6R	O3-C3-C2	-2.79	106.61	111.16
2	C	800	F6R	O3-C3-C2	-2.26	107.47	111.16
2	C	800	F6R	O2P-P-O3P	2.12	117.37	110.44
2	D	800	F6R	C1-C2-C3	2.07	120.18	116.26
2	B	800	F6R	O1P-P-O6	-2.04	101.03	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	352/376 (93%)	0.59	38 (10%) 6 10	28, 44, 69, 76	0
1	B	351/376 (93%)	0.94	56 (15%) 3 4	34, 59, 79, 85	0
1	C	352/376 (93%)	0.33	18 (5%) 27 37	22, 37, 58, 66	0
1	D	350/376 (93%)	0.16	7 (2%) 62 72	20, 33, 51, 55	0
All	All	1405/1504 (93%)	0.50	119 (8%) 11 17	20, 41, 73, 85	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	VAL	8.9
1	A	685	ASP	5.9
1	C	688	PHE	5.9
1	A	613	ARG	5.5
1	A	628	VAL	5.3
1	A	646	ILE	5.0
1	A	643	THR	4.9
1	B	341	SER	4.9
1	B	342	PHE	4.8
1	B	646	ILE	4.7
1	B	617	TYR	4.4
1	B	647	LYS	4.4
1	B	489	GLY	4.4
1	B	678	LEU	4.3
1	A	631	GLN	4.2
1	A	644	GLU	4.2
1	B	613	ARG	4.1
1	C	546	GLN	3.9
1	A	647	LYS	3.9
1	C	339	PHE	3.8
1	B	680	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	629	ALA	3.7
1	B	648	ASN	3.6
1	B	649	THR	3.6
1	B	340	SER	3.6
1	A	339	PHE	3.6
1	B	484	ALA	3.6
1	C	685	ASP	3.5
1	C	680	VAL	3.5
1	A	686	VAL	3.5
1	B	642	ASP	3.4
1	B	679	ALA	3.4
1	A	641	GLU	3.4
1	A	342	PHE	3.4
1	B	645	THR	3.3
1	A	684	TYR	3.3
1	A	388	ILE	3.3
1	B	552	LEU	3.3
1	C	342	PHE	3.2
1	C	689	PRO	3.2
1	A	338	ASN	3.2
1	A	490	VAL	3.2
1	A	642	ASP	3.1
1	B	686	VAL	3.1
1	A	648	ASN	3.1
1	B	657	HIS	3.0
1	A	340	SER	3.0
1	B	683	GLY	3.0
1	B	676	PHE	3.0
1	B	488	ILE	3.0
1	B	685	ASP	3.0
1	A	365	ASP	3.0
1	B	643	THR	2.9
1	A	617	TYR	2.9
1	B	640	LYS	2.9
1	A	415[A]	MET	2.9
1	C	613	ARG	2.9
1	A	680	VAL	2.8
1	B	687	ASP	2.8
1	B	550	THR	2.8
1	B	658	SER	2.8
1	C	554	HIS	2.8
1	B	491	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	611	ILE	2.8
1	B	628	VAL	2.7
1	C	686	VAL	2.7
1	D	367	TYR	2.7
1	B	543	ASP	2.7
1	B	582	TYR	2.6
1	C	490	VAL	2.6
1	A	367	TYR	2.6
1	B	547	LYS	2.5
1	A	599	ALA	2.5
1	A	609	MET	2.5
1	B	633	ARG	2.5
1	C	491	ALA	2.5
1	B	553	TYR	2.5
1	B	603	LYS	2.5
1	A	336	LYS	2.4
1	B	359	ARG	2.4
1	C	582	TYR	2.4
1	C	681	LEU	2.4
1	A	435	CYS	2.4
1	A	387	LEU	2.4
1	A	337	GLY	2.4
1	B	352	GLU	2.4
1	B	624	LEU	2.4
1	B	621	GLN	2.4
1	D	615	HIS	2.3
1	B	388	ILE	2.3
1	B	611	ILE	2.3
1	D	631	GLN	2.3
1	B	414	VAL	2.3
1	B	387	LEU	2.3
1	B	601	VAL	2.3
1	B	650	LYS	2.3
1	B	684	TYR	2.3
1	D	613	ARG	2.3
1	C	580	ILE	2.2
1	B	681	LEU	2.2
1	B	434	VAL	2.2
1	B	554	HIS	2.2
1	C	684	TYR	2.2
1	B	486	PRO	2.2
1	C	543	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	2.1
1	A	626	GLN	2.1
1	D	467	THR	2.1
1	A	526	LEU	2.1
1	A	612	MET	2.1
1	B	339	PHE	2.1
1	C	603	LYS	2.1
1	D	485	GLY	2.1
1	A	650	LYS	2.1
1	B	580	ILE	2.1
1	D	642	ASP	2.1
1	A	645	THR	2.0
1	A	654	LYS	2.0
1	B	570[A]	CYS	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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	F6R	C	800	16/16	0.14	-0.06	29,31,33,34	0
2	F6R	B	800	16/16	0.17	-0.17	44,48,51,52	0
2	F6R	D	800	16/16	0.13	-0.23	28,30,32,33	0
2	F6R	A	800	16/16	0.13	-0.32	38,40,41,41	0
3	CL	C	1691	1/1	0.07	-2.07	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.