



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:12 pm BST

PDB ID : 6NLH
Title : Structure of human triose phosphate isomerase R189A
Authors : Richards, K.R.; Roland, B.P.; Palladino, M.J.; VanDemark, A.P.
Deposited on : 2019-01-08
Resolution : 2.20 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 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	:	2.11
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)	:	2.11

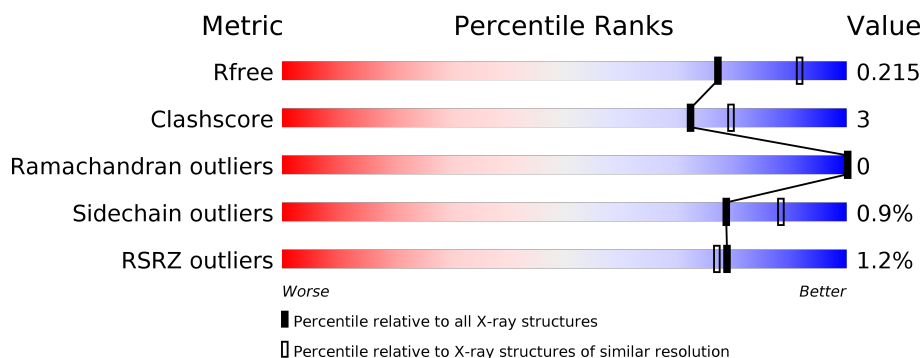
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	245	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
1	B	245	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	C	245	<div> <div>0%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	245	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	E	245	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>•</div> <div>•</div> </div> </div>
1	F	245	<div> <div>0%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	245	<div><div>%</div><div><div></div></div><div>91%9%</div></div>
1	H	245	<div><div>%</div><div><div></div></div><div>89%9%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29986 atoms, of which 14602 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	H	N	O	S	0	0	0
			3671	1161	1838	314	351	7			
1	E	238	Total	C	H	N	O	S	0	0	0
			3589	1137	1795	307	343	7			
1	B	245	Total	C	H	N	O	S	0	0	0
			3695	1167	1851	318	352	7			
1	C	239	Total	C	H	N	O	S	0	0	0
			3612	1143	1807	311	344	7			
1	D	245	Total	C	H	N	O	S	0	0	0
			3695	1167	1851	318	352	7			
1	F	239	Total	C	H	N	O	S	0	0	0
			3612	1143	1807	311	344	7			
1	G	245	Total	C	H	N	O	S	0	0	0
			3695	1167	1851	318	352	7			
1	H	239	Total	C	H	N	O	S	0	0	0
			3603	1141	1802	308	345	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	ALA	ARG	engineered mutation	UNP P60174
E	189	ALA	ARG	engineered mutation	UNP P60174
B	189	ALA	ARG	engineered mutation	UNP P60174
C	189	ALA	ARG	engineered mutation	UNP P60174
D	189	ALA	ARG	engineered mutation	UNP P60174
F	189	ALA	ARG	engineered mutation	UNP P60174
G	189	ALA	ARG	engineered mutation	UNP P60174
H	189	ALA	ARG	engineered mutation	UNP P60174

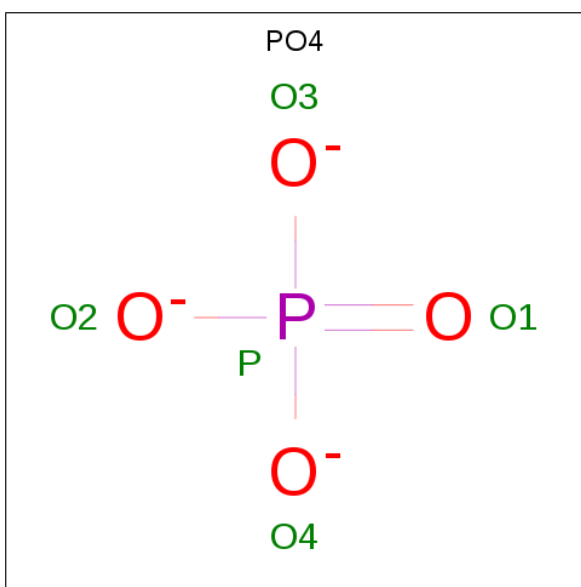
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	D	3	Total Na 3 3	0	0
2	E	1	Total Na 1 1	0	0
2	H	2	Total Na 2 2	0	0
2	B	4	Total Na 4 4	0	0
2	C	3	Total Na 3 3	0	0
2	A	3	Total Na 3 3	0	0
2	F	2	Total Na 2 2	0	0

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Br 1 1	0	0
3	C	1	Total Br 1 1	0	0
3	F	1	Total Br 1 1	0	0
3	E	1	Total Br 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

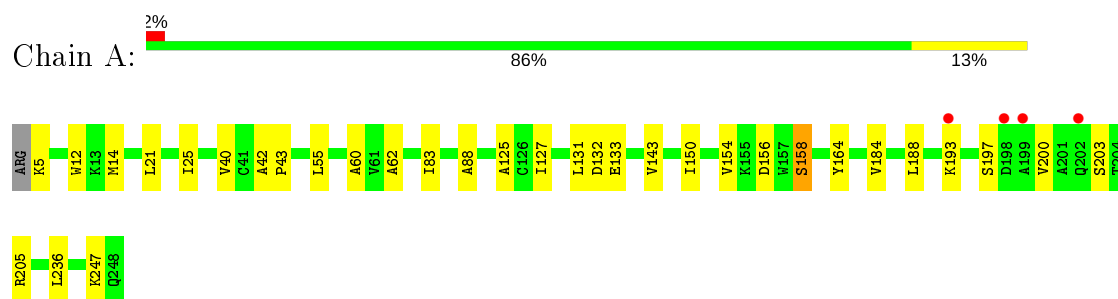
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		
5	E	79	Total	O	0	0
			79	79		
5	B	114	Total	O	0	0
			114	114		
5	C	86	Total	O	0	0
			86	86		
5	D	97	Total	O	0	0
			97	97		
5	F	85	Total	O	0	0
			85	85		
5	G	106	Total	O	0	0
			106	106		
5	H	85	Total	O	0	0
			85	85		

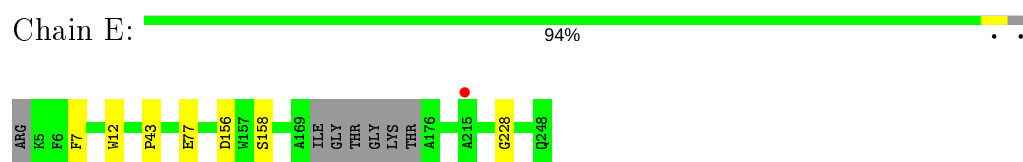
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

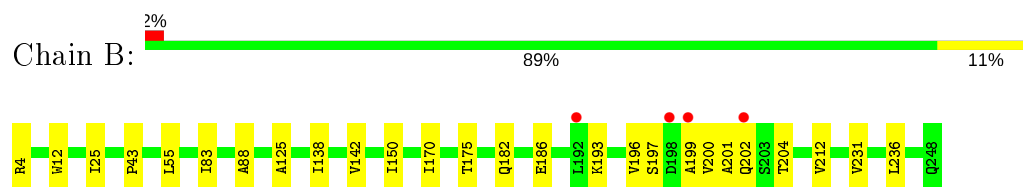
- Molecule 1: Triosephosphate isomerase



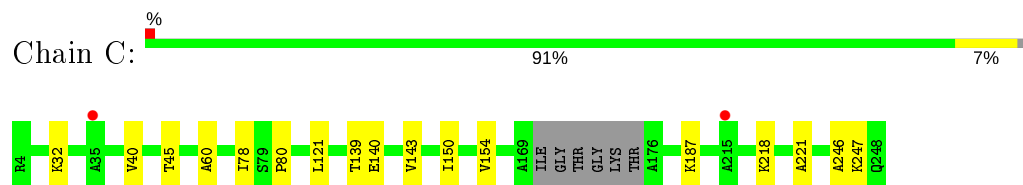
- Molecule 1: Triosephosphate isomerase



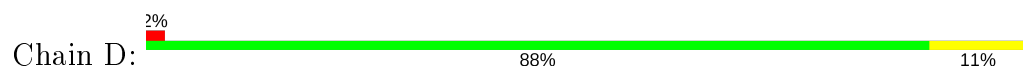
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase

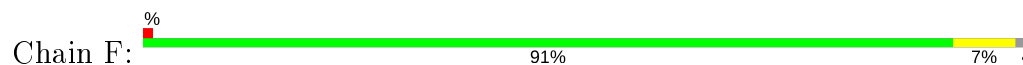


- Molecule 1: Triosephosphate isomerase





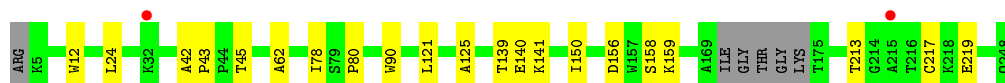
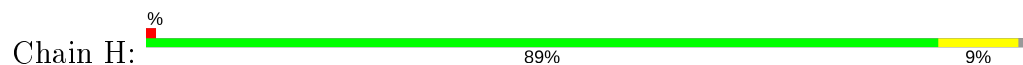
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.14Å 73.66Å 92.84Å 90.03° 90.03° 90.00°	Depositor
Resolution (Å)	19.66 – 2.20 34.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.66-2.20) 90.7 (34.24-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.174 , 0.216 0.175 , 0.215	Depositor DCC
R_{free} test set	1237 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l 0.477 for -h,k,-l 0.478 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29986	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, BR

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	0.46	0/1867	0.58	0/2529
1	B	0.48	0/1878	0.59	0/2543
1	C	0.41	0/1838	0.57	0/2488
1	D	0.47	0/1878	0.57	0/2543
1	E	0.41	0/1827	0.58	0/2474
1	F	0.42	0/1838	0.57	0/2488
1	G	0.46	0/1878	0.58	0/2543
1	H	0.44	0/1834	0.58	0/2484
All	All	0.44	0/14838	0.58	0/20092

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	1833	1838	1837	20	0
1	B	1844	1851	1851	16	0
1	C	1805	1807	1806	8	0
1	D	1844	1851	1851	16	0
1	E	1794	1795	1793	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1805	1807	1806	10	0
1	G	1844	1851	1851	14	0
1	H	1801	1802	1800	12	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	118	0	0	0	0
5	B	114	0	0	1	0
5	C	86	0	0	0	0
5	D	97	0	0	2	0
5	E	79	0	0	0	0
5	F	85	0	0	0	0
5	G	106	0	0	0	0
5	H	85	0	0	0	0
All	All	15384	14602	14595	99	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 3.

All (99) 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:143:VAL:CG1	1:A:188:LEU:HD21	2.17	0.74
1:G:143:VAL:CG1	1:G:188:LEU:HD21	2.22	0.69
1:A:127:ILE:HD12	1:A:143:VAL:HG13	1.80	0.64
1:H:125:ALA:HB1	1:H:150:ILE:HD13	1.84	0.60
1:E:156:ASP:OD1	1:E:158:SER:HB3	2.05	0.56
1:F:141:LYS:HD2	1:F:141:LYS:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:HG23	1:D:88:ALA:HB3	1.89	0.55
1:C:40:VAL:HG22	1:C:60:ALA:HB3	1.89	0.55
1:G:83:ILE:HG23	1:G:88:ALA:HB3	1.87	0.55
1:B:83:ILE:HG23	1:B:88:ALA:HB3	1.90	0.54
1:D:166:PRO:O	1:D:170:ILE:HD13	2.10	0.52
1:H:24:LEU:HD23	1:H:24:LEU:O	2.09	0.52
1:B:12:TRP:HB3	1:B:236:LEU:HD21	1.92	0.52
1:F:5:LYS:HD2	1:F:38:GLU:HB2	1.93	0.51
1:G:25:ILE:HG23	1:G:55:LEU:HD23	1.92	0.50
1:A:12:TRP:HB3	1:A:236:LEU:HD21	1.93	0.50
1:B:125:ALA:HB1	1:B:150:ILE:HD13	1.93	0.50
1:B:138:ILE:O	1:B:142:VAL:HG23	2.11	0.50
1:G:196:VAL:CG1	1:G:200:VAL:HG21	2.41	0.50
1:C:139:THR:O	1:C:143:VAL:HG22	2.11	0.50
1:D:12:TRP:CZ3	1:D:43:PRO:HB3	2.48	0.49
1:F:7:PHE:O	1:F:228:GLY:HA3	2.13	0.49
1:F:45:THR:HG23	1:F:78:ILE:HD13	1.95	0.48
1:B:4:ARG:NH1	1:B:204:THR:O	2.46	0.48
1:A:12:TRP:CZ3	1:A:43:PRO:HB3	2.49	0.48
1:B:83:ILE:CG2	1:B:88:ALA:HB3	2.43	0.48
1:B:12:TRP:CZ3	1:B:43:PRO:HB3	2.48	0.48
1:F:12:TRP:CZ3	1:F:43:PRO:HB3	2.49	0.48
1:B:170:ILE:HD11	5:B:483:HOH:O	2.13	0.48
1:G:196:VAL:HG11	1:G:200:VAL:HG21	1.95	0.47
1:A:14:MET:HG3	1:E:77:GLU:O	2.15	0.47
1:H:45:THR:HG23	1:H:78:ILE:HD13	1.97	0.47
1:A:83:ILE:HG23	1:A:88:ALA:HB3	1.96	0.46
1:A:150:ILE:O	1:A:154:VAL:HG23	2.16	0.46
1:C:80:PRO:HB3	1:C:121:LEU:HD12	1.97	0.46
1:A:83:ILE:CG2	1:A:88:ALA:HB3	2.45	0.46
1:D:212:VAL:HG11	1:D:231:VAL:HG22	1.97	0.46
1:D:213:THR:HB	1:D:239:GLU:OE2	2.16	0.46
1:H:156:ASP:HB3	1:H:159:LYS:HD3	1.97	0.46
1:H:80:PRO:HB3	1:H:121:LEU:HD12	1.97	0.46
1:F:125:ALA:HB1	1:F:150:ILE:HD13	1.98	0.46
1:B:25:ILE:HG23	1:B:55:LEU:HD23	1.99	0.45
1:A:143:VAL:HG13	1:A:188:LEU:HD21	1.98	0.45
1:B:193:LYS:CA	1:B:201:ALA:HB2	2.46	0.45
1:D:170:ILE:HG22	1:D:170:ILE:O	2.15	0.45
1:D:140:GLU:OE1	1:D:187:LYS:HD3	2.16	0.45
1:G:212:VAL:HG11	1:G:231:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:TRP:HB3	1:G:236:LEU:HD21	1.97	0.45
1:B:196:VAL:HG11	1:B:200:VAL:HG11	1.98	0.45
1:C:221:ALA:HB1	1:C:247:LYS:HD3	1.99	0.44
1:F:141:LYS:HD2	1:F:141:LYS:C	2.38	0.44
1:C:218:LYS:HG2	1:C:246:ALA:O	2.17	0.44
1:A:200:VAL:HA	1:A:203:SER:OG	2.17	0.44
1:A:25:ILE:HG23	1:A:55:LEU:HD23	1.99	0.44
1:B:182:GLN:NE2	1:B:186:GLU:HG3	2.32	0.44
1:B:212:VAL:HG11	1:B:231:VAL:HG22	1.98	0.44
1:B:193:LYS:HA	1:B:201:ALA:HB2	2.00	0.44
1:F:165:GLU:O	1:F:167:VAL:N	2.51	0.44
1:A:193:LYS:O	1:A:193:LYS:HD3	2.17	0.43
1:H:139:THR:HG23	1:H:140:GLU:N	2.33	0.43
1:C:150:ILE:O	1:C:154:VAL:HG23	2.18	0.43
1:D:4:ARG:HD3	1:D:202:GLN:O	2.18	0.43
1:D:63:ALA:HB2	1:D:83:ILE:HG12	2.00	0.43
1:G:138:ILE:O	1:G:142:VAL:HG23	2.18	0.43
1:B:175:THR:HG23	5:D:431:HOH:O	2.18	0.43
1:B:199:ALA:HA	1:B:202:GLN:HG2	1.99	0.43
1:A:40:VAL:HG22	1:A:60:ALA:HB3	2.01	0.43
1:D:114:ALA:HB2	1:D:153:ASN:HB3	2.01	0.43
1:D:50:PHE:CE1	1:D:54:LYS:HE2	2.53	0.43
1:D:83:ILE:CG2	1:D:88:ALA:HB3	2.48	0.43
1:H:12:TRP:CZ3	1:H:43:PRO:HB3	2.54	0.43
1:A:131:LEU:C	1:A:131:LEU:HD13	2.39	0.43
1:F:25:ILE:HG23	1:F:55:LEU:HD23	2.01	0.43
1:G:83:ILE:CG2	1:G:88:ALA:HB3	2.49	0.42
1:A:42:ALA:HA	1:A:62:ALA:O	2.19	0.42
1:C:45:THR:HG23	1:C:78:ILE:HD13	2.01	0.42
1:G:4:ARG:NH1	1:G:204:THR:O	2.52	0.42
1:H:156:ASP:OD1	1:H:158:SER:HB3	2.20	0.42
1:D:125:ALA:HB1	1:D:150:ILE:HD13	2.01	0.42
1:D:186:GLU:HG3	1:D:225:ASP:OD2	2.19	0.42
1:A:156:ASP:OD1	1:A:158:SER:HB3	2.20	0.42
1:C:140:GLU:OE2	1:C:187:LYS:HD3	2.20	0.42
1:D:196:VAL:HG12	1:D:197:SER:N	2.34	0.42
1:D:237:LYS:HE3	5:D:440:HOH:O	2.19	0.41
1:H:24:LEU:HD23	1:H:24:LEU:C	2.40	0.41
1:E:12:TRP:CZ3	1:E:43:PRO:HB3	2.55	0.41
1:E:7:PHE:O	1:E:228:GLY:HA3	2.20	0.41
1:G:125:ALA:HB1	1:G:150:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ALA:HB2	1:H:90:TRP:HB2	2.01	0.41
1:A:164:TYR:CE1	1:A:184:VAL:HG11	2.55	0.41
1:F:80:PRO:HB3	1:F:121:LEU:HD12	2.02	0.41
1:A:132:ASP:OD1	1:A:133:GLU:N	2.53	0.41
1:A:12:TRP:CE3	1:A:21:LEU:HD22	2.56	0.41
1:A:125:ALA:HB1	1:A:150:ILE:HD13	2.03	0.41
1:G:63:ALA:HB2	1:G:83:ILE:HG12	2.03	0.40
1:G:213:THR:HB	1:G:239:GLU:OE1	2.21	0.40
1:G:234:ALA:HA	1:G:237:LYS:HD2	2.03	0.40
1:H:213:THR:O	1:H:217:CYS:HB3	2.20	0.40
1:H:42:ALA:HA	1:H:62:ALA:O	2.21	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	242/245 (99%)	234 (97%)	8 (3%)	0	100	100
1	B	243/245 (99%)	238 (98%)	5 (2%)	0	100	100
1	C	235/245 (96%)	228 (97%)	7 (3%)	0	100	100
1	D	243/245 (99%)	237 (98%)	6 (2%)	0	100	100
1	E	234/245 (96%)	225 (96%)	9 (4%)	0	100	100
1	F	235/245 (96%)	227 (97%)	8 (3%)	0	100	100
1	G	243/245 (99%)	237 (98%)	6 (2%)	0	100	100
1	H	235/245 (96%)	225 (96%)	10 (4%)	0	100	100
All	All	1910/1960 (97%)	1851 (97%)	59 (3%)	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	191/192 (100%)	186 (97%)	5 (3%)	46	58
1	B	192/192 (100%)	191 (100%)	1 (0%)	88	94
1	C	188/192 (98%)	187 (100%)	1 (0%)	88	94
1	D	192/192 (100%)	188 (98%)	4 (2%)	53	67
1	E	187/192 (97%)	187 (100%)	0	100	100
1	F	188/192 (98%)	188 (100%)	0	100	100
1	G	192/192 (100%)	192 (100%)	0	100	100
1	H	188/192 (98%)	186 (99%)	2 (1%)	73	85
All	All	1518/1536 (99%)	1505 (99%)	13 (1%)	78	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	158	SER
1	A	197	SER
1	A	205	ARG
1	A	247	LYS
1	B	197	SER
1	C	32	LYS
1	D	158	SER
1	D	197	SER
1	D	198	ASP
1	D	205	ARG
1	H	141	LYS
1	H	219	GLU

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

Mol	Chain	Res	Type
1	E	202	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 24 are 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	$\# Z > 2$
4	PO4	C	305	-	4,4,4	0.67	0	6,6,6	0.47	0
4	PO4	H	304	-	4,4,4	0.84	0	6,6,6	0.49	0
4	PO4	F	304	-	4,4,4	0.71	0	6,6,6	0.61	0
4	PO4	E	303	-	4,4,4	0.87	0	6,6,6	0.40	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.

No monomer is involved in short contacts.

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	244/245 (99%)	-0.40	4 (1%) 72 70	14, 29, 55, 80	0
1	B	245/245 (100%)	-0.46	4 (1%) 72 70	15, 30, 55, 83	0
1	C	239/245 (97%)	-0.37	2 (0%) 86 85	17, 35, 59, 70	0
1	D	245/245 (100%)	-0.46	5 (2%) 65 63	15, 30, 54, 80	0
1	E	238/245 (97%)	-0.36	1 (0%) 92 91	16, 34, 61, 71	0
1	F	239/245 (97%)	-0.39	3 (1%) 77 75	16, 36, 63, 73	0
1	G	245/245 (100%)	-0.51	2 (0%) 86 85	14, 29, 55, 74	0
1	H	239/245 (97%)	-0.34	2 (0%) 86 85	16, 35, 61, 71	0
All	All	1934/1960 (98%)	-0.41	23 (1%) 79 77	14, 32, 60, 83	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	ALA	6.2
1	D	199	ALA	5.5
1	A	202	GLN	4.3
1	B	198	ASP	3.9
1	F	35	ALA	3.8
1	E	215	ALA	3.7
1	D	202	GLN	3.7
1	A	199	ALA	3.7
1	B	199	ALA	3.6
1	F	215	ALA	3.5
1	C	35	ALA	2.8
1	A	198	ASP	2.7
1	D	198	ASP	2.6
1	H	215	ALA	2.5
1	B	202	GLN	2.5
1	H	32	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	202	GLN	2.3
1	A	193	LYS	2.3
1	B	192	LEU	2.2
1	D	190	GLY	2.1
1	D	192	LEU	2.1
1	G	198	ASP	2.0
1	F	131	LEU	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 carbohydrates 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	NA	B	302	1/1	0.75	0.19	65,65,65,65	0
4	PO4	H	304	5/5	0.85	0.22	91,91,91,92	0
4	PO4	C	305	5/5	0.86	0.17	71,71,72,72	0
4	PO4	F	304	5/5	0.88	0.15	72,72,73,73	0
4	PO4	E	303	5/5	0.90	0.12	82,83,83,83	0
3	BR	C	304	1/1	0.91	0.10	77,77,77,77	0
2	NA	H	302	1/1	0.92	0.10	44,44,44,44	0
2	NA	F	301	1/1	0.94	0.09	37,37,37,37	0
2	NA	E	301	1/1	0.94	0.11	42,42,42,42	0
2	NA	C	301	1/1	0.95	0.30	48,48,48,48	0
2	NA	C	302	1/1	0.96	0.12	35,35,35,35	0
2	NA	C	303	1/1	0.96	0.06	30,30,30,30	0
3	BR	H	303	1/1	0.96	0.07	73,73,73,73	0
2	NA	A	303	1/1	0.97	0.09	36,36,36,36	0
2	NA	A	301	1/1	0.97	0.10	38,38,38,38	0
3	BR	E	302	1/1	0.97	0.07	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	A	302	1/1	0.97	0.27	38,38,38,38	0
2	NA	H	301	1/1	0.97	0.06	32,32,32,32	0
2	NA	D	303	1/1	0.97	0.07	37,37,37,37	0
3	BR	F	303	1/1	0.98	0.07	80,80,80,80	0
2	NA	B	304	1/1	0.98	0.07	45,45,45,45	0
2	NA	D	302	1/1	0.98	0.05	27,27,27,27	0
2	NA	G	302	1/1	0.98	0.10	33,33,33,33	0
2	NA	G	301	1/1	0.98	0.19	32,32,32,32	0
2	NA	B	303	1/1	0.98	0.08	35,35,35,35	0
2	NA	D	301	1/1	0.99	0.14	39,39,39,39	0
2	NA	F	302	1/1	0.99	0.08	31,31,31,31	0
2	NA	B	301	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.