



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:16 PM UTC

PDB ID : 3CRV / pdb_00003crv
Title : XPD_Helicase
Authors : Fan, L.; Arvai, A.S.; Tainer, J.A.
Deposited on : 2008-04-07
Resolution : 2.00 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

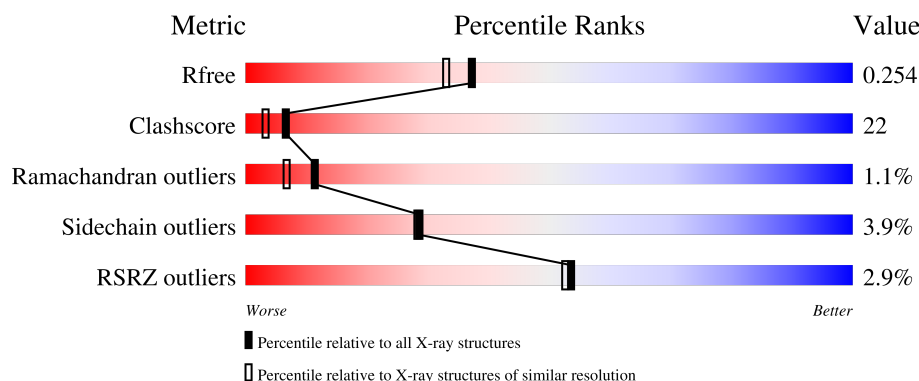
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

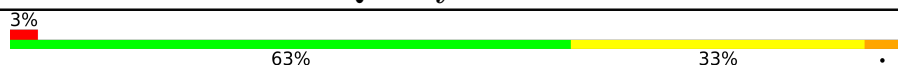
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	551	

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	FLC	A	1900	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IPA	A	1811	-	-	X	-
5	GOL	A	2000	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4819 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.

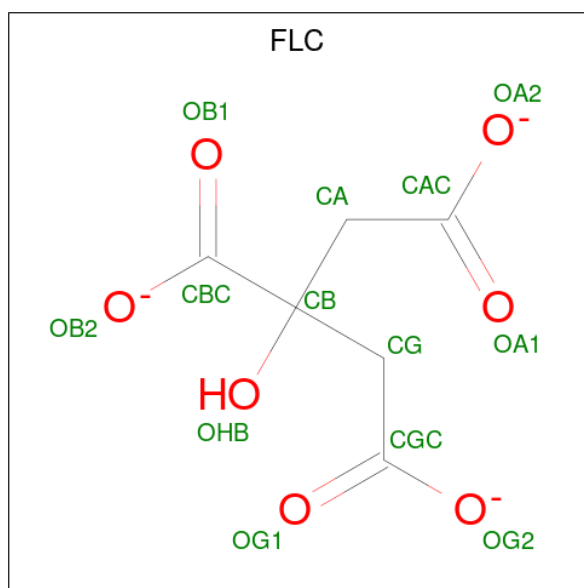
- Molecule 1 is a protein called XPD/Rad3 related DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4505	2902	750	834	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

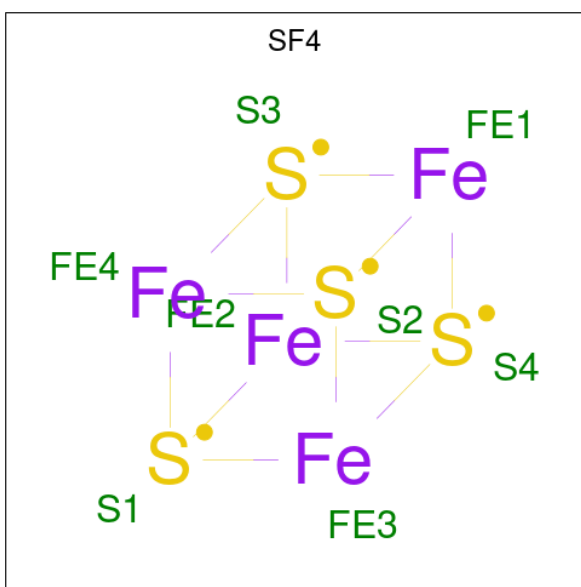
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q4JC68

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



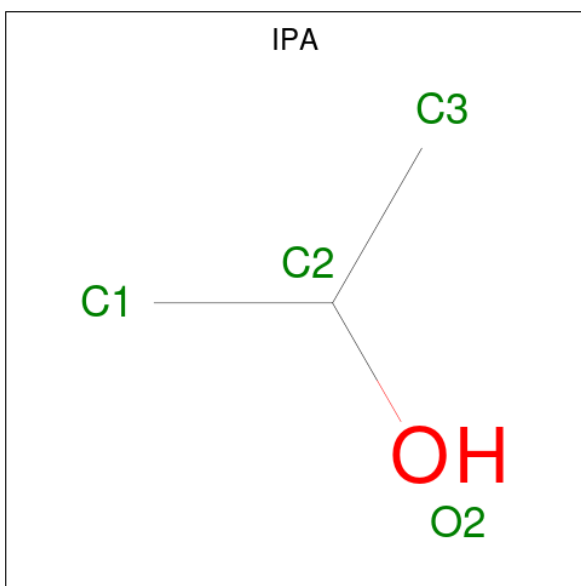
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



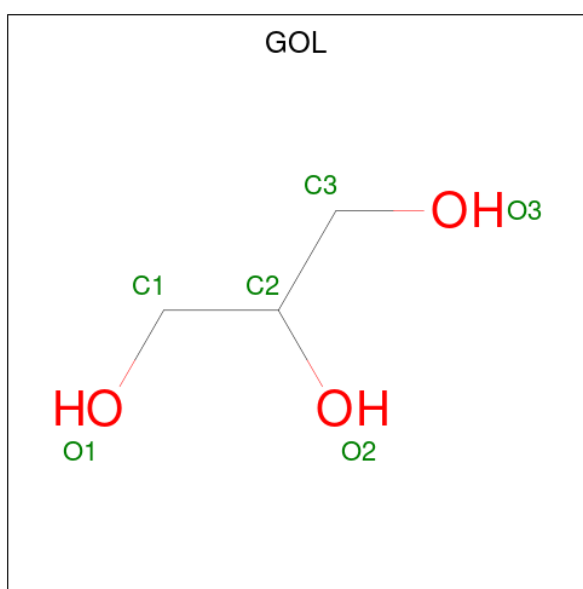
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

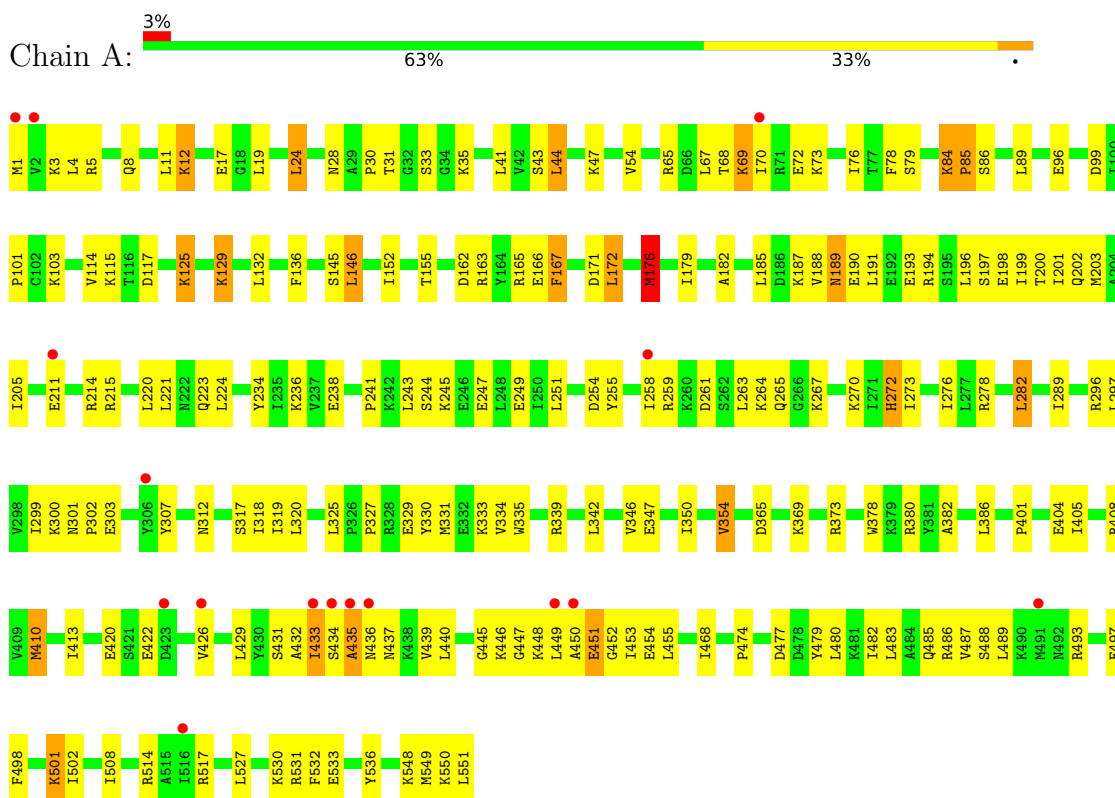
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	259	Total	O	0	0
			259	259		

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: XPD/Rad3 related DNA helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.54Å 70.22Å 144.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.58 – 2.00 42.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.58-2.00) 93.5 (42.58-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.260 0.214 , 0.254	Depositor DCC
R_{free} test set	3498 reflections (9.43%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4819	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: GOL, FLC, IPA, SF4

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	0.40	1/4587 (0.0%)	0.92	17/6179 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	LYS	C-O	-6.32	1.16	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CA-C-N	-12.77	106.59	119.87
1	A	84	LYS	C-N-CA	-12.77	106.59	119.87
1	A	318	ILE	N-CA-C	7.43	119.54	108.46
1	A	85	PRO	N-CA-C	-7.38	104.95	114.03
1	A	176	MET	N-CA-C	-7.22	97.47	109.46
1	A	272	HIS	N-CA-C	6.58	119.30	111.33
1	A	47	LYS	CA-C-N	6.56	126.00	118.85
1	A	47	LYS	C-N-CA	6.56	126.00	118.85
1	A	474	PRO	N-CA-C	-6.51	102.75	110.70
1	A	501	LYS	N-CA-C	6.10	118.01	111.36
1	A	354	VAL	N-CA-C	-5.88	107.26	112.90
1	A	346	VAL	N-CA-C	5.85	116.50	110.36
1	A	301	ASN	CA-C-N	5.85	125.52	119.56
1	A	301	ASN	C-N-CA	5.85	125.52	119.56
1	A	146	LEU	N-CA-C	5.51	117.75	111.02
1	A	549	MET	N-CA-C	5.41	117.06	108.79
1	A	24	LEU	N-CA-C	-5.14	101.59	109.76

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	4505	0	4651	189	0
2	A	13	0	5	8	0
3	A	8	0	0	0	0
4	A	28	0	56	10	0
5	A	6	0	8	8	0
6	A	259	0	0	7	1
All	All	4819	0	4720	200	1

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 22.

All (200) 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:198:GLU:HG3	1:A:221:LEU:HD11	1.35	1.06
2:A:1900:FLC:OA1	2:A:1900:FLC:HG2	1.63	0.96
4:A:1811:IPA:H11	5:A:2000:GOL:H31	1.51	0.93
1:A:373:ARG:HH22	5:A:2000:GOL:H32	1.34	0.91
1:A:531:ARG:HH12	4:A:1811:IPA:H31	1.36	0.90
1:A:451:GLU:H	1:A:514:ARG:HH21	1.21	0.87
1:A:196:LEU:HD21	1:A:201:ILE:HD11	1.57	0.87
1:A:531:ARG:HH12	4:A:1811:IPA:C3	1.88	0.87
1:A:41:LEU:HD13	1:A:70:ILE:HD11	1.58	0.84
1:A:303:GLU:HG3	1:A:486:ARG:HB3	1.63	0.81
1:A:487:VAL:HG12	1:A:489:LEU:HD13	1.61	0.80
1:A:451:GLU:N	1:A:514:ARG:HH21	1.79	0.80
1:A:422:GLU:HA	1:A:448:LYS:NZ	1.98	0.79
1:A:30:PRO:HG3	1:A:354:VAL:HG23	1.65	0.79
1:A:199:ILE:HG12	1:A:203:MET:HE2	1.65	0.79
1:A:194:ARG:HG2	1:A:282:LEU:HD12	1.69	0.75
1:A:125:LYS:HE3	1:A:125:LYS:HA	1.70	0.74
1:A:245:LYS:O	1:A:249:GLU:HG3	1.88	0.74
1:A:189:ASN:HD22	1:A:190:GLU:N	1.87	0.73
1:A:531:ARG:NH1	4:A:1811:IPA:H31	2.04	0.73
1:A:69:LYS:O	1:A:69:LYS:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:HA	1:A:165:ARG:NH1	2.04	0.72
2:A:1900:FLC:OA1	2:A:1900:FLC:CG	2.30	0.71
1:A:189:ASN:HD22	1:A:190:GLU:H	1.38	0.71
1:A:1:MET:HG2	1:A:41:LEU:HD21	1.73	0.70
1:A:422:GLU:HA	1:A:448:LYS:HZ1	1.58	0.69
1:A:487:VAL:HG12	1:A:487:VAL:O	1.93	0.69
1:A:255:TYR:CZ	1:A:259:ARG:HD2	2.29	0.67
1:A:453:ILE:CD1	1:A:514:ARG:HH22	2.07	0.67
1:A:410:MET:CE	1:A:440:LEU:HD13	2.25	0.67
1:A:289:ILE:HD12	1:A:302:PRO:HG2	1.77	0.67
1:A:211:GLU:HA	1:A:214:ARG:HE	1.60	0.66
1:A:531:ARG:HH22	4:A:1811:IPA:H31	1.61	0.66
1:A:162:ASP:HA	1:A:165:ARG:HH12	1.60	0.65
1:A:188:VAL:HG13	1:A:191:LEU:HD12	1.78	0.65
1:A:455:LEU:HG	1:A:514:ARG:HH12	1.60	0.65
1:A:365:ASP:HB2	1:A:380:ARG:NH2	2.12	0.65
1:A:244:SER:OG	1:A:247:GLU:HG3	1.97	0.64
1:A:236:LYS:HE2	1:A:238:GLU:OE2	1.97	0.64
1:A:373:ARG:NH2	5:A:2000:GOL:H32	2.11	0.64
1:A:365:ASP:HB2	1:A:380:ARG:HH21	1.63	0.63
1:A:445:GLY:C	1:A:447:GLY:H	2.05	0.63
1:A:468:ILE:CD1	1:A:508:ILE:HG23	2.28	0.63
1:A:426:VAL:HG11	1:A:453:ILE:HG21	1.81	0.63
1:A:194:ARG:HB2	1:A:299:ILE:HD11	1.80	0.62
1:A:224:LEU:HD13	1:A:224:LEU:O	1.98	0.62
1:A:410:MET:HE1	1:A:440:LEU:HD13	1.80	0.62
1:A:451:GLU:HA	1:A:514:ARG:HE	1.64	0.61
2:A:1900:FLC:OG1	2:A:1900:FLC:CBC	2.44	0.61
1:A:482:ILE:O	1:A:485:GLN:HG2	2.01	0.60
1:A:211:GLU:N	1:A:214:ARG:HH21	1.99	0.60
1:A:483:LEU:HD23	1:A:483:LEU:C	2.28	0.59
1:A:129:LYS:N	1:A:129:LYS:HE3	2.17	0.59
1:A:404:GLU:HG2	1:A:405:ILE:N	2.18	0.58
1:A:454:GLU:HG2	1:A:517:ARG:HH12	1.68	0.58
1:A:5:ARG:H	1:A:8:GLN:NE2	2.02	0.58
1:A:289:ILE:HD13	1:A:482:ILE:HD13	1.85	0.58
1:A:329:GLU:HB3	1:A:498:PHE:HZ	1.69	0.57
1:A:468:ILE:HD11	1:A:508:ILE:HG23	1.85	0.57
1:A:99:ASP:O	1:A:101:PRO:HD3	2.03	0.57
1:A:103:LYS:HG3	6:A:822:HOH:O	2.05	0.57
1:A:187:LYS:HA	1:A:187:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HG3	1:A:486:ARG:CB	2.33	0.57
1:A:468:ILE:HD12	1:A:527:LEU:HD23	1.86	0.56
1:A:114:VAL:HG22	1:A:145:SER:HB3	1.86	0.56
1:A:373:ARG:HH22	5:A:2000:GOL:C3	2.10	0.56
1:A:166:GLU:HG3	1:A:167:PHE:N	2.21	0.56
1:A:198:GLU:HG3	1:A:221:LEU:CD1	2.25	0.56
1:A:19:LEU:HD11	1:A:319:ILE:HD11	1.88	0.56
1:A:176:MET:HE1	1:A:319:ILE:HG13	1.87	0.56
1:A:347:GLU:CG	1:A:354:VAL:HG22	2.35	0.56
1:A:197:SER:HB3	1:A:296:ARG:HG2	1.88	0.56
1:A:451:GLU:CB	4:A:1812:IPA:H33	2.36	0.56
1:A:493:ARG:HE	1:A:493:ARG:HA	1.69	0.56
1:A:4:LEU:HD22	1:A:4:LEU:N	2.21	0.55
1:A:378:TRP:NE1	1:A:408:ARG:HD2	2.22	0.55
1:A:531:ARG:NH2	4:A:1811:IPA:H31	2.21	0.55
1:A:429:LEU:O	1:A:433:ILE:HG12	2.07	0.55
1:A:497:GLU:HA	1:A:501:LYS:HB2	1.89	0.55
1:A:224:LEU:HD13	1:A:224:LEU:C	2.32	0.54
1:A:488:SER:O	1:A:489:LEU:HD12	2.08	0.54
4:A:1811:IPA:H11	5:A:2000:GOL:C3	2.32	0.54
1:A:453:ILE:C	1:A:453:ILE:HD12	2.33	0.54
1:A:453:ILE:HD11	1:A:514:ARG:HH22	1.72	0.54
1:A:30:PRO:CG	1:A:354:VAL:HG23	2.37	0.53
1:A:382:ALA:O	1:A:386:LEU:HD13	2.07	0.53
1:A:445:GLY:O	1:A:447:GLY:N	2.41	0.53
5:A:2000:GOL:H12	6:A:680:HOH:O	2.07	0.53
1:A:450:ALA:C	1:A:452:GLY:H	2.16	0.53
1:A:410:MET:HE3	1:A:413:ILE:HD12	1.91	0.53
1:A:194:ARG:CG	1:A:282:LEU:HD12	2.36	0.52
1:A:265:GLN:O	1:A:267:LYS:HG3	2.09	0.52
1:A:401:PRO:HB2	5:A:2000:GOL:H2	1.92	0.52
1:A:28:ASN:ND2	1:A:325:LEU:H	2.07	0.52
1:A:487:VAL:O	1:A:487:VAL:CG1	2.57	0.52
1:A:263:LEU:HD13	1:A:263:LEU:O	2.09	0.52
1:A:480:LEU:HD23	1:A:480:LEU:O	2.09	0.51
1:A:501:LYS:HD3	1:A:536:TYR:CZ	2.46	0.51
1:A:24:LEU:C	1:A:24:LEU:HD23	2.36	0.51
1:A:300:LYS:HD3	1:A:479:TYR:CE1	2.45	0.51
1:A:450:ALA:HB1	1:A:453:ILE:HG13	1.93	0.51
1:A:453:ILE:HD12	1:A:453:ILE:O	2.11	0.51
1:A:193:GLU:OE2	1:A:300:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:O	1:A:185:LEU:HG	2.11	0.51
1:A:251:LEU:HD22	1:A:273:ILE:HD11	1.92	0.51
1:A:31:THR:HA	1:A:35:LYS:HE2	1.92	0.50
1:A:73:LYS:HD2	1:A:73:LYS:N	2.26	0.50
1:A:211:GLU:HA	1:A:214:ARG:NE	2.26	0.50
1:A:501:LYS:HD3	1:A:536:TYR:CE2	2.46	0.50
1:A:451:GLU:HB2	4:A:1812:IPA:H33	1.93	0.50
1:A:115:LYS:HE2	1:A:117:ASP:HB3	1.93	0.50
1:A:432:ALA:C	1:A:434:SER:H	2.20	0.49
1:A:550:LYS:O	1:A:551:LEU:HB2	2.12	0.49
2:A:1900:FLC:OA1	2:A:1900:FLC:CBC	2.53	0.49
2:A:1900:FLC:OA1	2:A:1900:FLC:OB2	2.29	0.49
1:A:171:ASP:O	1:A:172:LEU:CB	2.60	0.49
2:A:1900:FLC:OG1	2:A:1900:FLC:OB1	2.30	0.49
1:A:369:LYS:HE2	2:A:1900:FLC:OB2	2.13	0.49
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.77	0.49
1:A:447:GLY:O	1:A:448:LYS:HB3	2.13	0.49
1:A:448:LYS:HG2	1:A:448:LYS:O	2.12	0.49
2:A:1900:FLC:OB2	2:A:1900:FLC:CAC	2.59	0.49
1:A:404:GLU:HG2	1:A:405:ILE:H	1.78	0.48
1:A:5:ARG:H	1:A:8:GLN:HE21	1.60	0.48
1:A:350:ILE:HD11	1:A:354:VAL:HG13	1.95	0.48
1:A:72:GLU:HG3	1:A:76:ILE:CD1	2.44	0.48
1:A:101:PRO:CG	1:A:263:LEU:HB2	2.44	0.48
1:A:426:VAL:HG13	1:A:453:ILE:HG12	1.95	0.48
1:A:429:LEU:C	1:A:429:LEU:HD13	2.39	0.47
1:A:488:SER:C	1:A:489:LEU:HD12	2.39	0.47
1:A:468:ILE:HD13	1:A:508:ILE:HG23	1.96	0.47
1:A:445:GLY:C	1:A:447:GLY:N	2.71	0.47
1:A:533:GLU:OE1	1:A:548:LYS:HD2	2.14	0.47
1:A:96:GLU:OE1	1:A:270:LYS:HE2	2.14	0.47
1:A:12:LYS:HB3	1:A:12:LYS:NZ	2.30	0.47
1:A:72:GLU:HG3	1:A:76:ILE:HD11	1.97	0.47
1:A:435:ALA:N	6:A:800:HOH:O	2.48	0.47
1:A:163:ARG:HG3	6:A:806:HOH:O	2.14	0.47
1:A:317:SER:HA	6:A:637:HOH:O	2.14	0.46
1:A:450:ALA:HB1	1:A:453:ILE:CG1	2.45	0.46
1:A:189:ASN:ND2	1:A:190:GLU:N	2.59	0.46
1:A:482:ILE:HA	1:A:485:GLN:HG2	1.97	0.46
1:A:30:PRO:HG2	1:A:33:SER:HB3	1.97	0.46
1:A:436:ASN:O	1:A:437:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HG23	1:A:214:ARG:HG2	1.97	0.46
1:A:531:ARG:CZ	4:A:1811:IPA:H31	2.44	0.46
1:A:188:VAL:HG11	1:A:307:TYR:HB3	1.97	0.45
1:A:223:GLN:HE21	1:A:241:PRO:HB3	1.81	0.45
1:A:312:ASN:HA	1:A:339:ARG:HD2	1.98	0.45
1:A:261:ASP:O	1:A:264:LYS:HB2	2.17	0.45
1:A:67:LEU:O	1:A:70:ILE:HG22	2.17	0.45
1:A:101:PRO:HG3	1:A:263:LEU:HB2	1.98	0.45
1:A:165:ARG:HG2	6:A:662:HOH:O	2.17	0.44
1:A:84:LYS:O	1:A:85:PRO:C	2.54	0.44
1:A:437:ASN:O	1:A:439:VAL:HG23	2.17	0.44
1:A:455:LEU:HG	1:A:514:ARG:NH1	2.31	0.44
1:A:41:LEU:CD1	1:A:70:ILE:HD11	2.39	0.44
1:A:420:GLU:HB2	1:A:449:LEU:HD22	1.99	0.44
1:A:198:GLU:O	1:A:202:GLN:HG3	2.17	0.44
1:A:255:TYR:CE2	1:A:259:ARG:HD2	2.53	0.44
1:A:28:ASN:HD22	1:A:325:LEU:HB2	1.82	0.43
1:A:54:VAL:O	1:A:155:THR:HA	2.18	0.43
1:A:165:ARG:HB3	1:A:165:ARG:HH11	1.83	0.43
5:A:2000:GOL:C1	6:A:680:HOH:O	2.66	0.43
1:A:234:TYR:O	1:A:477:ASP:HB2	2.18	0.43
1:A:527:LEU:HB3	1:A:532:PHE:CD1	2.53	0.43
1:A:136:PHE:CD1	1:A:136:PHE:C	2.96	0.43
1:A:333:LYS:HD2	1:A:333:LYS:N	2.32	0.43
1:A:179:ILE:HD12	1:A:320:LEU:CD2	2.49	0.43
1:A:433:ILE:HG22	1:A:439:VAL:HB	2.01	0.43
1:A:263:LEU:HD13	1:A:263:LEU:C	2.43	0.42
1:A:67:LEU:HD23	1:A:78:PHE:HB2	2.01	0.42
1:A:386:LEU:HD11	1:A:413:ILE:HG12	2.01	0.42
1:A:84:LYS:C	1:A:86:SER:N	2.76	0.42
1:A:69:LYS:HE2	1:A:69:LYS:HB2	1.77	0.42
1:A:166:GLU:HG3	1:A:167:PHE:H	1.84	0.42
1:A:79:SER:O	1:A:152:ILE:HA	2.20	0.42
1:A:179:ILE:HD12	1:A:320:LEU:HD21	2.02	0.42
1:A:273:ILE:HA	1:A:276:ILE:HD12	2.02	0.42
1:A:408:ARG:HG2	1:A:408:ARG:HH21	1.85	0.42
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.86	0.42
1:A:211:GLU:OE1	1:A:215:ARG:NH2	2.53	0.41
1:A:254:ASP:O	1:A:258:ILE:HG13	2.20	0.41
1:A:289:ILE:HD12	1:A:302:PRO:CG	2.49	0.41
1:A:327:PRO:HD2	1:A:502:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG23	1:A:200:THR:N	2.35	0.41
1:A:431:SER:O	1:A:434:SER:N	2.53	0.41
1:A:480:LEU:HD23	1:A:480:LEU:C	2.45	0.41
1:A:330:TYR:CE1	1:A:334:VAL:HG21	2.56	0.41
1:A:114:VAL:HG22	1:A:145:SER:CB	2.50	0.41
1:A:331:MET:HG2	1:A:335:TRP:CE3	2.55	0.41
1:A:171:ASP:O	1:A:172:LEU:HB2	2.21	0.41
1:A:187:LYS:HD3	1:A:190:GLU:OE1	2.20	0.41
1:A:43:SER:HA	1:A:176:MET:HG3	2.03	0.41
1:A:194:ARG:CZ	1:A:278:ARG:HD2	2.51	0.41
1:A:203:MET:HB3	1:A:272:HIS:CD2	2.56	0.41
1:A:65:ARG:O	1:A:68:THR:HG22	2.21	0.41
1:A:1:MET:SD	1:A:12:LYS:HE3	2.61	0.40
1:A:194:ARG:HB2	1:A:299:ILE:CD1	2.47	0.40
1:A:410:MET:HE3	1:A:413:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:616:HOH:O	6:A:720:HOH:O[3_545]	2.10	0.10

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	549/551 (100%)	518 (94%)	25 (5%)	6 (1%)	11 7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	LYS

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Mol	Chain	Res	Type
1	A	3	LYS
1	A	172	LEU
1	A	433	ILE
1	A	435	ALA
1	A	451	GLU

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	511/511 (100%)	491 (96%)	20 (4%)	28	28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	LYS
1	A	17	GLU
1	A	44	LEU
1	A	69	LYS
1	A	89	LEU
1	A	125	LYS
1	A	129	LYS
1	A	132	LEU
1	A	146	LEU
1	A	167	PHE
1	A	176	MET
1	A	189	ASN
1	A	220	LEU
1	A	243	LEU
1	A	282	LEU
1	A	297	LEU
1	A	342	LEU
1	A	410	MET
1	A	530	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	21	ASN
1	A	22	ASN
1	A	28	ASN
1	A	75	ASN
1	A	189	ASN
1	A	222	ASN
1	A	223	GLN
1	A	269	ASN
1	A	314	ASN
1	A	458	ASN
1	A	520	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](#)

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](#)

10 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	$\# Z > 2$
3	SF4	A	600	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	A	1900	-	12,12,12	1.94	3 (25%)	17,17,17	3.37	9 (52%)
4	IPA	A	1810	-	3,3,3	0.52	0	3,3,3	0.34	0
4	IPA	A	1811	-	3,3,3	0.51	0	3,3,3	0.33	0
4	IPA	A	1808	-	3,3,3	0.61	0	3,3,3	0.34	0
4	IPA	A	1807	-	3,3,3	0.60	0	3,3,3	0.33	0
4	IPA	A	1806	-	3,3,3	0.61	0	3,3,3	0.33	0
4	IPA	A	1812	-	3,3,3	0.52	0	3,3,3	0.34	0
5	GOL	A	2000	-	5,5,5	0.32	0	5,5,5	0.25	0
4	IPA	A	1804	-	3,3,3	0.50	0	3,3,3	0.87	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
3	SF4	A	600	1	-	-	0/6/5/5
5	GOL	A	2000	-	-	2/4/4/4	-
2	FLC	A	1900	-	-	3/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1900	FLC	OA2-CAC	-3.96	1.17	1.30
2	A	1900	FLC	OB2-CBC	-3.54	1.17	1.30
2	A	1900	FLC	OA1-CAC	-2.58	1.13	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1900	FLC	OB2-CBC-CB	6.05	124.74	113.14
2	A	1900	FLC	OHB-CB-CBC	5.10	116.19	108.96
2	A	1900	FLC	OA2-CAC-CA	4.95	130.04	114.35
2	A	1900	FLC	CB-CA-CAC	-4.48	101.67	113.92
2	A	1900	FLC	OB2-CBC-OB1	-4.46	109.59	123.86
2	A	1900	FLC	OA2-CAC-OA1	-4.22	112.48	123.33
2	A	1900	FLC	OG1-CGC-CG	-3.79	112.21	122.95
2	A	1900	FLC	OHB-CB-CG	-3.71	100.90	109.38
2	A	1900	FLC	OG2-CGC-CG	2.50	122.28	114.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2000	GOL	C1-C2-C3-O3
5	A	2000	GOL	O2-C2-C3-O3
2	A	1900	FLC	CAC-CA-CB-OHB
2	A	1900	FLC	CG-CB-CBC-OB2
2	A	1900	FLC	CA-CB-CBC-OB2

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1900	FLC	8	0
4	A	1811	IPA	8	0
4	A	1812	IPA	2	0
5	A	2000	GOL	8	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	551/551 (100%)	0.33	16 (2%) 53 52	19, 40, 68, 84	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.5
1	A	449	LEU	3.5
1	A	516	ILE	2.9
1	A	433	ILE	2.8
1	A	426	VAL	2.7
1	A	2	VAL	2.5
1	A	70	ILE	2.5
1	A	434	SER	2.4
1	A	423	ASP	2.3
1	A	436	ASN	2.3
1	A	450	ALA	2.3
1	A	211	GLU	2.2
1	A	258	ILE	2.1
1	A	491	MET	2.0
1	A	306	TYR	2.0
1	A	435	ALA	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 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($\text{\AA}^2$)	Q<0.9
4	IPA	A	1810	4/4	0.42	0.25	66,67,67,67	0
4	IPA	A	1806	4/4	0.44	0.23	77,78,78,78	0
2	FLC	A	1900	13/13	0.61	0.14	53,61,63,64	0
4	IPA	A	1812	4/4	0.64	0.21	69,70,70,70	0
4	IPA	A	1811	4/4	0.68	0.23	55,56,57,58	0
5	GOL	A	2000	6/6	0.69	0.17	66,67,67,67	0
4	IPA	A	1808	4/4	0.72	0.19	76,76,76,76	0
4	IPA	A	1807	4/4	0.74	0.23	66,67,68,68	0
4	IPA	A	1804	4/4	0.78	0.20	67,68,69,69	0
3	SF4	A	600	8/8	0.99	0.03	36,38,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.