



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:02 PM UTC

PDB ID : 4XR5 / pdb_00004xr5
Title : X-ray structure of the unliganded thymidine phosphorylase from Salmonella typhimurium at 2.05 Å resolution
Authors : Balaev, V.V.; Lashkov, A.A.; Gabdulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on : 2015-01-20
Resolution : 2.05 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

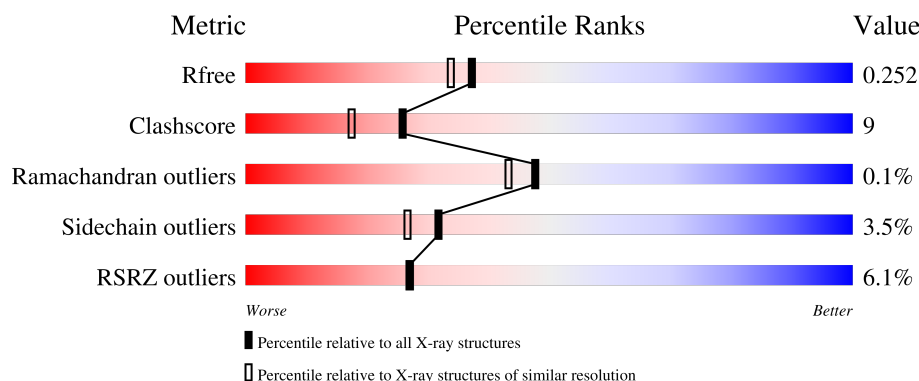
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	440	4% 81% 17% .
1	B	440	9% 71% 27% .

2 Entry composition [i](#)

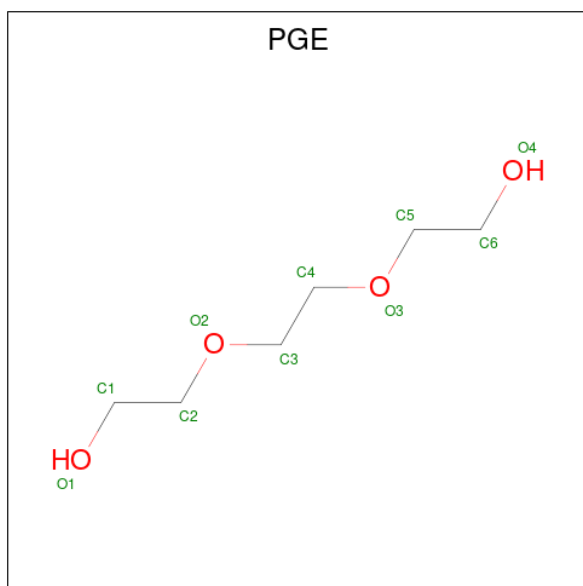
There are 5 unique types of molecules in this entry. The entry contains 6717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3291	2062	566	641	22			
1	B	440	Total	C	N	O	S	0	1	0
			3299	2066	567	644	22			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

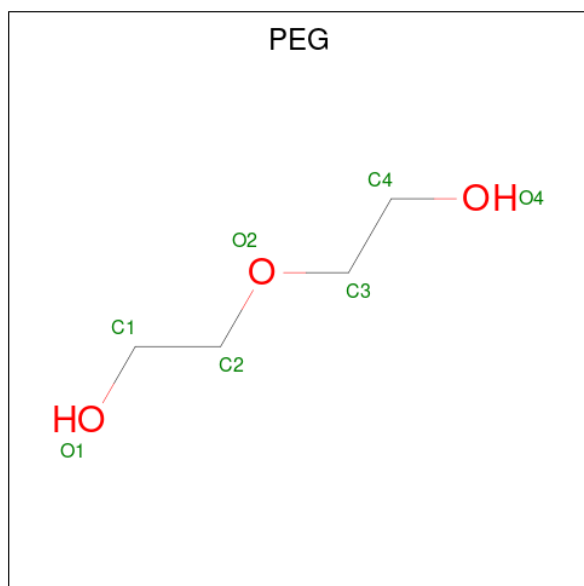


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 4 3	0	0

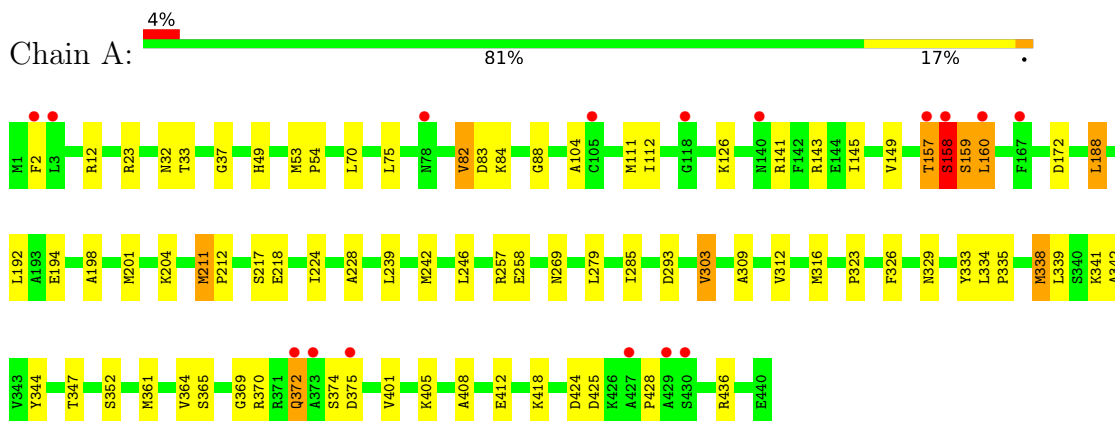
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	B	52	Total O 52 52	0	0

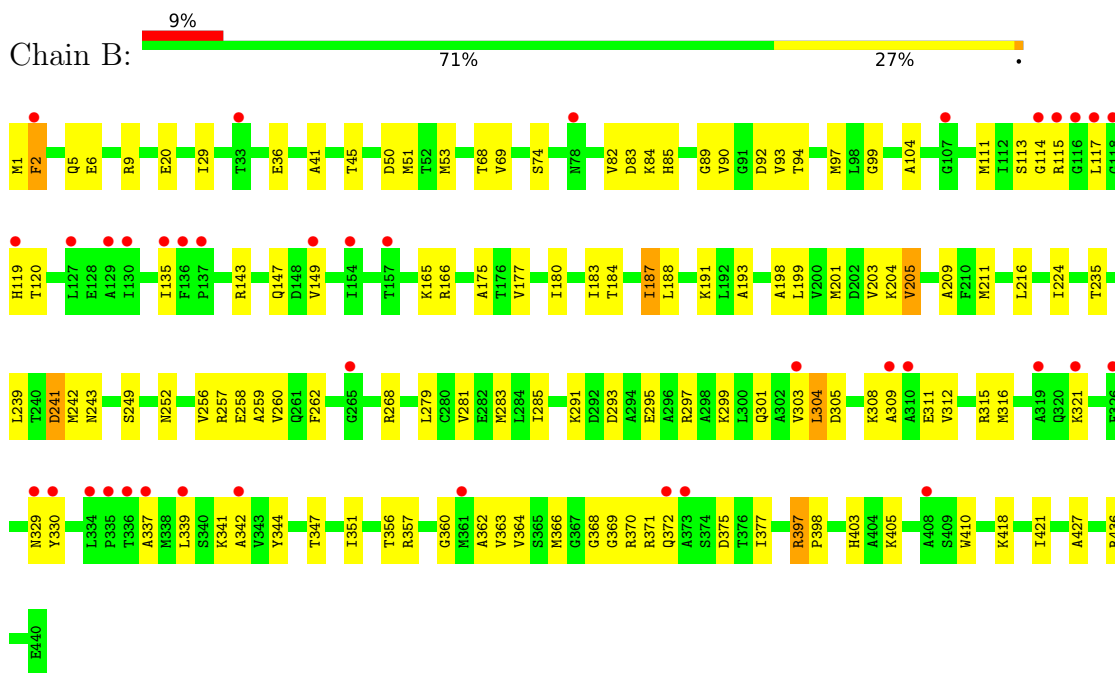
3 Residue-property plots [i](#)

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: Thymidine phosphorylase



• Molecule 1: Thymidine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.94Å 171.21Å 45.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.05 47.72 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.72-2.05) 95.5 (47.72-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9-1692	Depositor
R, R_{free}	0.221 , 0.247 0.230 , 0.252	Depositor DCC
R_{free} test set	2946 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: CL, PGE, PEG

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	0.58	0/3339	0.95	7/4514 (0.2%)
1	B	0.58	0/3347	1.02	13/4525 (0.3%)
All	All	0.58	0/6686	0.99	20/9039 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	GLY	CA-C-N	7.22	126.48	118.97
1	B	99	GLY	C-N-CA	7.22	126.48	118.97
1	B	397	ARG	CA-C-N	6.97	126.73	119.76
1	B	397	ARG	C-N-CA	6.97	126.73	119.76
1	B	329	ASN	N-CA-C	6.20	120.54	112.92
1	B	53	MET	CA-C-N	-6.12	112.70	119.19
1	B	53	MET	C-N-CA	-6.12	112.70	119.19
1	B	375	ASP	N-CA-C	5.67	118.18	110.35
1	A	157	THR	CB-CA-C	-5.64	101.43	110.79
1	B	321	LYS	N-CA-C	5.57	120.02	113.23
1	B	241	ASP	CA-C-N	-5.57	114.20	123.33
1	B	241	ASP	C-N-CA	-5.57	114.20	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	MET	CA-C-N	5.50	125.02	119.19
1	A	211	MET	C-N-CA	5.50	125.02	119.19
1	A	329	ASN	N-CA-C	5.50	118.99	112.72
1	A	160	LEU	N-CA-C	5.42	117.74	108.90
1	B	427	ALA	CA-C-N	-5.28	115.33	120.98
1	B	427	ALA	C-N-CA	-5.28	115.33	120.98
1	A	269	ASN	CA-C-N	5.09	124.88	119.28
1	A	269	ASN	C-N-CA	5.09	124.88	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	PHE	Peptide
1	B	2	PHE	Peptide

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	3291	0	3306	53	0
1	B	3299	0	3309	73	0
2	A	20	0	28	5	0
2	B	10	0	14	1	0
3	B	1	0	0	0	0
4	B	7	0	10	1	0
5	A	37	0	0	3	0
5	B	52	0	0	0	1
All	All	6717	0	6667	126	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 9.

All (126) 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:157:THR:O	1:A:158:SER:HB3	1.30	1.04
1:A:157:THR:OG1	1:A:159:SER:OG	1.88	0.89
1:A:372:GLN:HG2	1:A:375:ASP:N	1.89	0.88
1:A:372:GLN:HG2	1:A:375:ASP:H	1.34	0.88
1:A:157:THR:O	1:A:158:SER:CB	2.16	0.86
1:A:75:LEU:HD11	1:A:143:ARG:HG2	1.58	0.85
1:A:201:MET:HG3	1:A:224:ILE:HG21	1.59	0.84
1:B:201:MET:HG3	1:B:224:ILE:HG21	1.63	0.81
1:B:89:GLY:HA3	1:B:242:MET:HE3	1.66	0.76
1:B:364:VAL:HA	1:B:369:GLY:H	1.51	0.75
1:A:370:ARG:HB3	1:A:375:ASP:HB2	1.69	0.74
1:A:257:ARG:NH1	2:A:502:PGE:O1	2.20	0.74
1:A:12:ARG:NH1	1:B:175:ALA:O	2.25	0.69
1:A:239:LEU:HD12	1:A:436:ARG:HG2	1.74	0.69
1:B:303:VAL:HG13	1:B:308:LYS:HB2	1.75	0.69
1:A:352:SER:HA	1:A:428:PRO:HG3	1.76	0.67
1:A:23:ARG:NH1	5:A:601:HOH:O	2.22	0.66
1:A:84:LYS:NZ	5:A:607:HOH:O	2.30	0.65
1:A:339:LEU:HD11	1:A:341:LYS:HD2	1.77	0.65
1:B:342:ALA:HB1	1:B:398:PRO:HB3	1.78	0.65
1:A:157:THR:HG1	1:A:159:SER:HG	1.20	0.64
1:A:364:VAL:HG22	1:A:369:GLY:HA3	1.78	0.64
1:B:363:VAL:HG12	1:B:368:GLY:HA3	1.80	0.63
1:B:249:SER:OG	1:B:258:GLU:OE1	2.12	0.63
1:A:424:ASP:OD1	1:A:425:ASP:N	2.27	0.62
1:B:308:LYS:O	1:B:312:VAL:HG23	2.00	0.62
1:B:252:ASN:O	1:B:256:VAL:HG23	1.99	0.61
1:B:113:SER:OG	1:B:114:GLY:N	2.34	0.60
1:B:119:HIS:CG	1:B:357:ARG:HG2	2.37	0.60
1:B:104:ALA:HB2	1:B:312:VAL:HG21	1.82	0.59
1:B:311:GLU:HG2	1:B:315:ARG:HH11	1.67	0.58
1:B:119:HIS:O	1:B:360:GLY:HA3	2.03	0.58
1:B:241:ASP:OD2	1:B:243:ASN:ND2	2.32	0.58
1:B:93:VAL:HG21	1:B:259:ALA:HB2	1.86	0.58
1:A:211:MET:HG3	1:A:217:SER:HA	1.85	0.58
1:B:203:VAL:HB	1:B:239:LEU:HD23	1.87	0.57
1:A:344:TYR:O	1:A:418:LYS:HE3	2.04	0.57
1:B:143:ARG:O	1:B:147:GLN:HG3	2.05	0.56
1:A:303:VAL:HG13	1:A:309:ALA:HB2	1.88	0.55
1:B:360:GLY:O	1:B:364:VAL:HG23	2.08	0.54
1:A:323:PRO:HB2	1:A:326:PHE:HB2	1.90	0.54
1:B:341:LYS:HG3	1:B:410:TRP:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB3	1:A:242:MET:HB2	1.90	0.53
2:A:501:PGE:O4	2:A:501:PGE:H32	2.09	0.53
1:A:218:GLU:OE2	1:A:436:ARG:NH1	2.38	0.53
1:B:312:VAL:HA	1:B:315:ARG:HD3	1.90	0.52
1:B:239:LEU:HD12	1:B:436:ARG:HG2	1.91	0.52
1:A:112:ILE:HD12	1:A:194:GLU:HG2	1.91	0.52
1:A:104:ALA:HB2	1:A:312:VAL:HG21	1.92	0.52
1:B:362:ALA:O	1:B:366:MET:HG3	2.10	0.52
1:B:84:LYS:HD2	1:B:279:LEU:HD13	1.91	0.52
1:B:204:LYS:HD2	1:B:242:MET:HE2	1.91	0.51
1:A:342:ALA:HA	1:A:401:VAL:HA	1.91	0.51
1:A:84:LYS:HD2	1:A:279:LEU:HD13	1.91	0.51
1:B:268:ARG:CZ	1:B:304:LEU:HG	2.41	0.51
1:B:90:VAL:HG21	1:B:356:THR:O	2.11	0.51
1:B:205:VAL:HA	1:B:209:ALA:HB2	1.93	0.50
1:A:37:GLY:N	1:B:36:GLU:OE2	2.34	0.50
1:B:1:MET:HG3	1:B:2:PHE:H	1.76	0.50
1:A:338:MET:HE3	1:A:405:LYS:O	2.12	0.50
1:B:82:VAL:HG13	1:B:198:ALA:HB3	1.94	0.50
1:B:303:VAL:HG12	1:B:309:ALA:HB2	1.93	0.49
1:B:370:ARG:HB3	1:B:372:GLN:O	2.12	0.49
1:B:29:ILE:O	1:B:166:ARG:HD3	2.12	0.49
1:B:83:ASP:OD1	1:B:111:MET:HG3	2.13	0.49
1:A:83:ASP:OD1	1:A:111:MET:HG3	2.13	0.49
1:B:85:HIS:NE2	1:B:187:ILE:HG12	2.28	0.49
1:B:149:VAL:HG11	1:B:316:MET:HB2	1.95	0.48
1:A:12:ARG:O	1:A:49:HIS:NE2	2.44	0.48
1:B:97:MET:HG2	1:B:262:PHE:CD1	2.49	0.48
1:B:92:ASP:OD1	1:B:94:THR:HG23	2.14	0.47
1:B:337:ALA:CB	1:B:403:HIS:HB3	2.44	0.47
1:B:344:TYR:O	1:B:418:LYS:HE2	2.14	0.47
2:A:502:PGE:H32	2:A:502:PGE:H5	1.29	0.47
1:A:364:VAL:HG13	1:A:369:GLY:C	2.39	0.46
1:B:41:ALA:O	1:B:45:THR:HG23	2.16	0.46
1:B:69:VAL:HG13	1:B:193:ALA:HA	1.98	0.46
1:A:82:VAL:HG13	1:A:198:ALA:HB3	1.96	0.46
1:B:301:GLN:HE21	1:B:305[A]:ASP:CG	2.25	0.45
1:A:211:MET:HA	1:A:212:PRO:HD3	1.74	0.45
2:B:503:PGE:H22	2:B:503:PGE:H4	1.46	0.45
1:A:188:LEU:HD21	1:A:228:ALA:HB2	1.99	0.45
1:B:115:ARG:HH21	1:B:135:ILE:HD11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:NZ	5:A:621:HOH:O	2.50	0.45
1:B:180:ILE:HA	1:B:183:ILE:HD12	1.99	0.45
1:B:256:VAL:O	1:B:260:VAL:HG23	2.17	0.45
1:B:50:ASP:OD1	1:B:51:MET:N	2.50	0.45
1:B:191:LYS:HA	1:B:191:LYS:HD2	1.75	0.44
1:B:293:ASP:CG	1:B:297:ARG:HE	2.24	0.44
1:B:364:VAL:HA	1:B:369:GLY:N	2.24	0.44
1:B:281:VAL:O	1:B:285:ILE:HG13	2.18	0.44
1:A:53:MET:HB3	1:A:54:PRO:HD3	2.00	0.44
1:A:242:MET:HE1	1:A:246:LEU:HB2	2.00	0.44
1:B:6:GLU:OE1	1:B:9:ARG:NH1	2.51	0.43
1:A:285:ILE:HD11	1:A:293:ASP:N	2.33	0.43
1:B:199:LEU:O	1:B:235:THR:HA	2.18	0.43
1:B:257:ARG:HG3	1:B:330:TYR:CE1	2.54	0.43
1:A:149:VAL:HG11	1:A:316:MET:HB2	2.00	0.42
1:B:119:HIS:CD2	1:B:120:THR:HG23	2.54	0.42
1:B:370:ARG:NE	1:B:377:ILE:HG13	2.34	0.42
1:A:188:LEU:O	1:A:192:LEU:HG	2.19	0.42
1:A:372:GLN:NE2	1:A:374:SER:OG	2.53	0.42
1:B:397:ARG:HA	1:B:398:PRO:HD3	1.69	0.42
1:B:405:LYS:HB3	1:B:405:LYS:HE3	1.69	0.42
1:B:82:VAL:HG12	1:B:283:MET:HE3	2.01	0.42
1:A:88:GLY:O	1:A:204:LYS:HG3	2.20	0.41
1:A:258:GLU:HB2	2:A:502:PGE:C6	2.50	0.41
1:B:165:LYS:HE2	1:B:165:LYS:HB2	1.71	0.41
1:A:372:GLN:HG3	1:A:374:SER:H	1.84	0.41
1:B:89:GLY:HA2	1:B:120:THR:HG22	2.02	0.41
1:B:312:VAL:HA	1:B:315:ARG:CD	2.51	0.41
1:A:334:LEU:HA	1:A:335:PRO:HD3	1.99	0.41
1:B:119:HIS:ND1	1:B:357:ARG:HG2	2.36	0.41
1:B:211:MET:HA	1:B:211:MET:HE2	2.03	0.41
1:A:361:MET:HB2	1:A:361:MET:HE2	1.78	0.41
1:B:339:LEU:HD21	1:B:341:LYS:HE2	2.03	0.41
1:A:172:ASP:O	1:B:5:GLN:NE2	2.53	0.41
1:A:408:ALA:O	1:A:412:GLU:HG2	2.21	0.41
1:B:74:SER:HB3	4:B:502:PEG:H12	2.02	0.41
1:A:333:TYR:CZ	2:A:501:PGE:H6	2.56	0.40
1:B:184:THR:O	1:B:188:LEU:HB2	2.20	0.40
1:B:337:ALA:HB2	1:B:403:HIS:HB3	2.01	0.40
1:A:141:ARG:O	1:A:145:ILE:HG13	2.21	0.40
1:A:159:SER:HG	1:A:159:SER:H	1.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HG23	1:B:421:ILE:HG23	2.03	0.40
1:B:295:GLU:OE2	1:B:299:LYS:NZ	2.55	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)
5:B:601:HOH:O	5:B:601:HOH:O[2_655]	2.16	0.04

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	438/440 (100%)	425 (97%)	12 (3%)	1 (0%)	43	37
1	B	439/440 (100%)	433 (99%)	6 (1%)	0	100	100
All	All	877/880 (100%)	858 (98%)	18 (2%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	SER

5.3.2 Protein sidechains [i](#)

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	344/344 (100%)	331 (96%)	13 (4%)	29	24
1	B	345/344 (100%)	334 (97%)	11 (3%)	34	29
All	All	689/688 (100%)	665 (96%)	24 (4%)	32	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	THR
1	A	70	LEU
1	A	82	VAL
1	A	158	SER
1	A	159	SER
1	A	160	LEU
1	A	188	LEU
1	A	303	VAL
1	A	338	MET
1	A	347	THR
1	A	365	SER
1	A	372	GLN
1	B	20	GLU
1	B	68	THR
1	B	117	LEU
1	B	177	VAL
1	B	187	ILE
1	B	205	VAL
1	B	216	LEU
1	B	291	LYS
1	B	304	LEU
1	B	347	THR
1	B	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	243	ASN
1	A	372	GLN
1	B	301	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 oligosaccharides 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	PGE	B	503	-	9,9,9	0.29	0	8,8,8	0.37	0
2	PGE	A	502	-	9,9,9	0.28	0	8,8,8	0.83	0
2	PGE	A	501	-	9,9,9	0.37	0	8,8,8	0.25	0
4	PEG	B	502	-	6,6,6	0.58	0	5,5,5	0.55	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	PGE	B	503	-	-	4/7/7/7	-
2	PGE	A	502	-	-	4/7/7/7	-
2	PGE	A	501	-	-	5/7/7/7	-
4	PEG	B	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	PGE	C3-C4-O3-C5
2	A	501	PGE	C4-C3-O2-C2
2	B	503	PGE	C4-C3-O2-C2
2	A	501	PGE	O1-C1-C2-O2
2	A	501	PGE	O3-C5-C6-O4
2	A	501	PGE	O2-C3-C4-O3
2	B	503	PGE	O1-C1-C2-O2
4	B	502	PEG	O1-C1-C2-O2
2	B	503	PGE	O3-C5-C6-O4
4	B	502	PEG	O2-C3-C4-O4
2	A	501	PGE	C3-C4-O3-C5
2	A	502	PGE	O1-C1-C2-O2
2	B	503	PGE	C1-C2-O2-C3
2	A	502	PGE	O3-C5-C6-O4
2	A	502	PGE	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	PGE	1	0
2	A	502	PGE	3	0
2	A	501	PGE	2	0
4	B	502	PEG	1	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	440/440 (100%)	0.38	16 (3%)	46 46	36, 49, 68, 85	0
1	B	440/440 (100%)	0.70	38 (8%)	16 16	27, 51, 77, 91	1 (0%)
All	All	880/880 (100%)	0.54	54 (6%)	27 27	27, 50, 73, 91	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	GLY	4.1
1	B	117	LEU	4.1
1	A	2	PHE	4.0
1	B	118	GLY	3.7
1	B	137	PRO	3.6
1	A	157	THR	3.4
1	B	339	LEU	3.4
1	B	337	ALA	3.3
1	B	129	ALA	3.3
1	B	119	HIS	3.2
1	B	373	ALA	3.1
1	B	107	GLY	2.9
1	A	118	GLY	2.9
1	B	408	ALA	2.9
1	B	33	THR	2.8
1	A	430	SER	2.7
1	B	2	PHE	2.7
1	A	373	ALA	2.7
1	A	78	ASN	2.6
1	A	429	ALA	2.6
1	A	167	PHE	2.5
1	B	136	PHE	2.5
1	A	427	ALA	2.5
1	A	158	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	114	GLY	2.5
1	A	372	GLN	2.5
1	A	3	LEU	2.5
1	B	309	ALA	2.5
1	B	135	ILE	2.5
1	B	157	THR	2.4
1	A	160	LEU	2.3
1	B	321	LYS	2.3
1	B	335	PRO	2.3
1	B	130	ILE	2.3
1	B	330	TYR	2.3
1	B	303	VAL	2.3
1	B	326	PHE	2.2
1	B	334	LEU	2.2
1	B	336	THR	2.2
1	A	375	ASP	2.2
1	B	265	GLY	2.2
1	B	127	LEU	2.2
1	B	115	ARG	2.1
1	B	78	ASN	2.1
1	B	329	ASN	2.1
1	B	149	VAL	2.1
1	B	342	ALA	2.1
1	B	361	MET	2.1
1	B	319	ALA	2.1
1	B	154	ILE	2.1
1	B	310	ALA	2.1
1	A	140	ASN	2.0
1	A	105	CYS	2.0
1	B	372	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 oligosaccharides 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
2	PGE	A	501	10/10	0.80	0.14	52,63,67,69	0
2	PGE	A	502	10/10	0.81	0.13	51,53,55,56	0
2	PGE	B	503	10/10	0.81	0.13	62,66,73,74	0
4	PEG	B	502	7/7	0.82	0.11	55,57,67,69	0
3	CL	B	501	1/1	0.91	0.13	60,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.