



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 12:40 PM UTC

PDB ID : 4AH3 / pdb_00004ah3
Title : Crystal structure of the holo omega-transaminase from *Chromobacterium violaceum*
Authors : Sayer, C.; Isupov, M.N.; Littlechild, J.A.
Deposited on : 2012-02-03
Resolution : 1.57 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

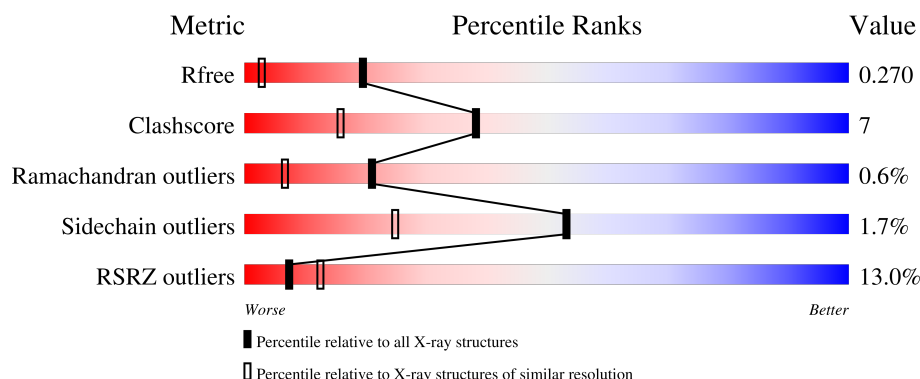
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	459	89% 10% .
1	B	459	8% 86% 12% ..
1	C	459	16% 83% 15% ..
1	D	459	26% 81% 17% ..

2 Entry composition [i](#)

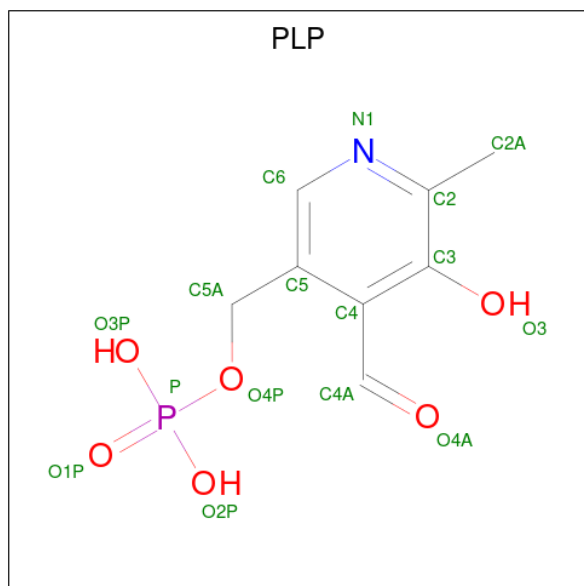
There are 3 unique types of molecules in this entry. The entry contains 16845 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMEGA-TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	36	0
			3785	2431	655	678	21			
1	B	455	Total	C	N	O	S	0	33	0
			3755	2406	654	673	22			
1	C	455	Total	C	N	O	S	0	23	0
			3706	2374	645	664	23			
1	D	454	Total	C	N	O	S	0	20	0
			3674	2347	641	663	23			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

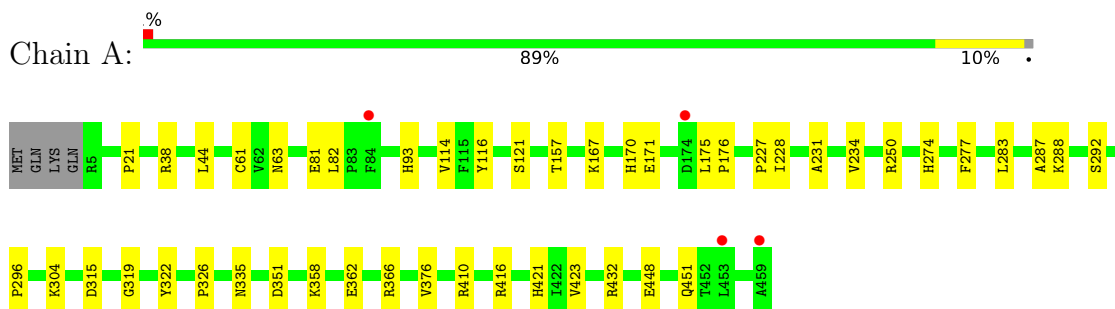
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	722	Total	O	0	0
			722	722		
3	B	560	Total	O	0	0
			560	560		
3	C	346	Total	O	0	0
			346	346		
3	D	237	Total	O	0	0
			237	237		

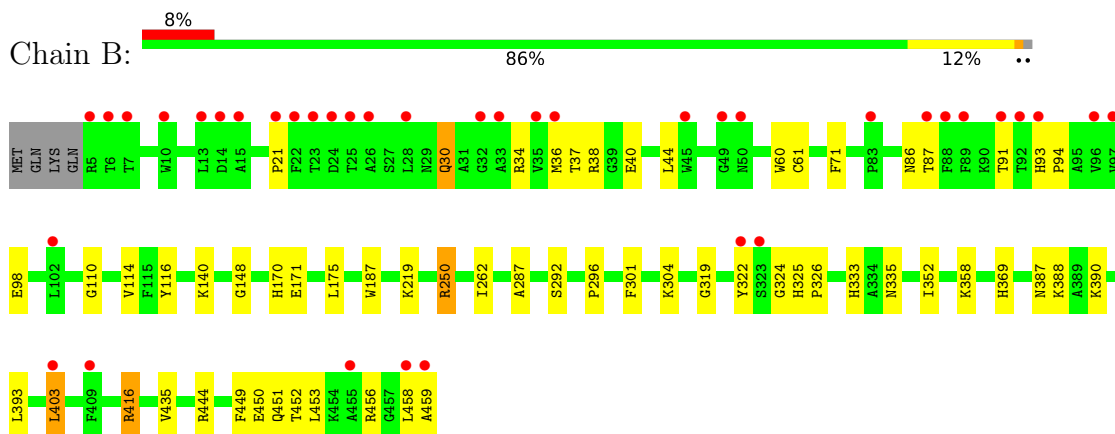
3 Residue-property plots [i](#)

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.

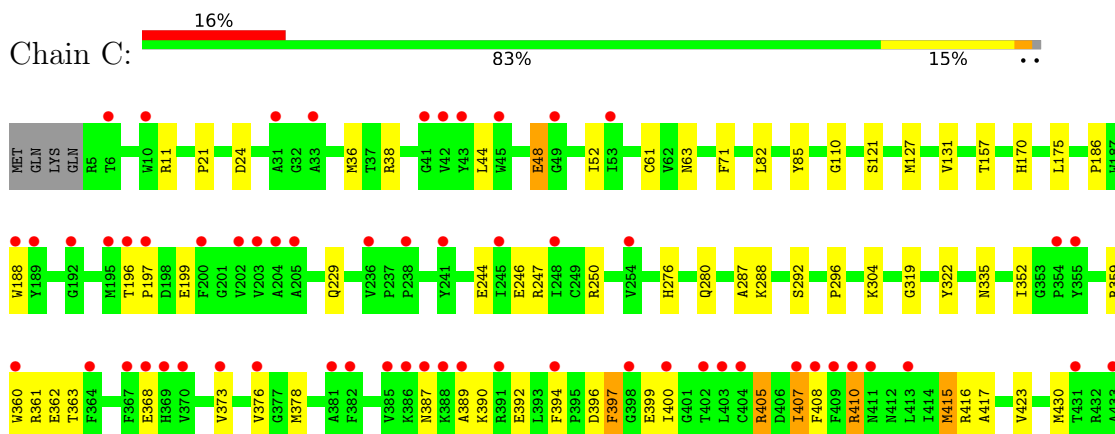
• Molecule 1: OMEGA-TRANSAMINASE

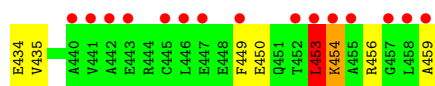


• Molecule 1: OMEGA-TRANSAMINASE

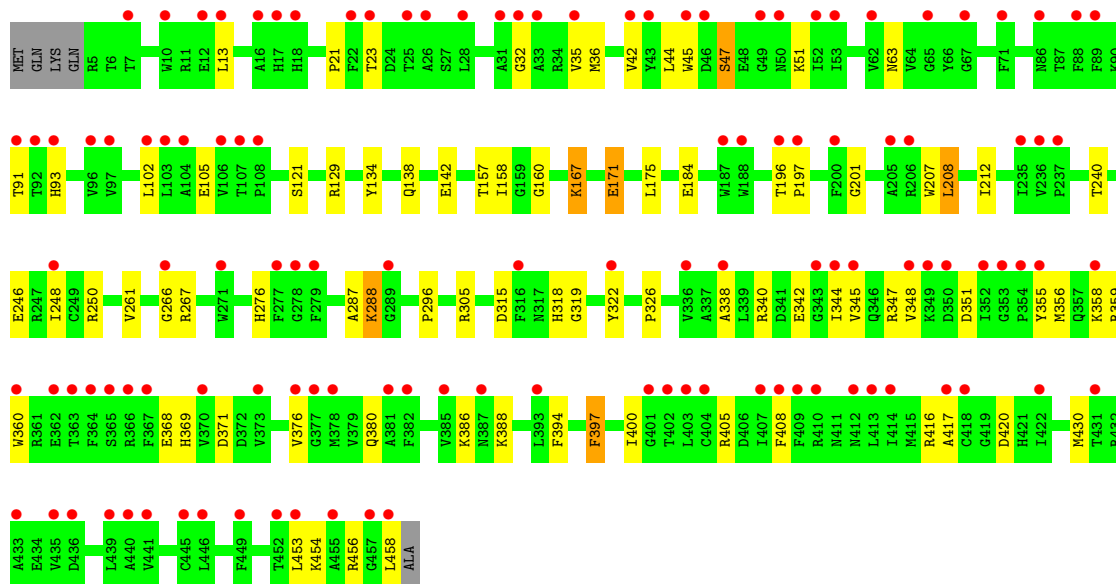
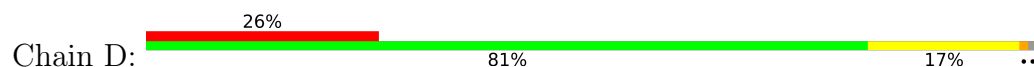


• Molecule 1: OMEGA-TRANSAMINASE





● Molecule 1: OMEGA-TRANSAMINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.89Å 62.23Å 119.61Å 75.14° 81.73° 76.17°	Depositor
Resolution (Å)	115.19 – 1.57 115.16 – 1.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (115.19-1.57) 94.4 (115.16-1.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.222 , 0.273 0.220 , 0.270	Depositor DCC
R_{free} test set	11003 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	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	16845	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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: PLP

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	1.00	3/3989 (0.1%)	1.04	2/5391 (0.0%)
1	B	0.86	0/3948	0.96	3/5332 (0.1%)
1	C	0.79	0/3871	0.92	2/5236 (0.0%)
1	D	0.72	0/3825	0.88	0/5173
All	All	0.85	3/15633 (0.0%)	0.95	7/21132 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	HIS	CG-CD2	6.34	1.42	1.35
1	A	170	HIS	CG-ND1	-5.92	1.31	1.38
1	A	274	HIS	ND1-CE1	5.03	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ARG	N-CA-C	5.66	117.13	111.07
1	C	63	ASN	N-CA-C	5.44	117.21	111.28
1	A	63	ASN	N-CA-C	5.24	117.73	111.71
1	A	335	ASN	N-CA-C	5.16	116.59	111.07
1	B	148	GLY	N-CA-C	-5.09	104.13	111.20
1	B	140	LYS	CA-C-N	5.07	125.14	119.87
1	B	140	LYS	C-N-CA	5.07	125.14	119.87

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	3785	0	3785	35	0
1	B	3755	0	3758	57	0
1	C	3706	0	3667	59	0
1	D	3674	0	3623	72	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	7	0	0
2	D	15	0	6	0	0
3	A	722	0	0	5	0
3	B	560	0	0	12	0
3	C	346	0	0	6	0
3	D	237	0	0	4	0
All	All	16845	0	14858	207	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 7.

All (207) 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:B:36[B]:MET:HE3	1:B:44:LEU:CD2	1.81	1.08
1:B:38[B]:ARG:CG	1:B:38[B]:ARG:HH11	1.67	1.05
1:A:228[B]:ILE:HD11	1:A:277:PHE:CZ	1.93	1.04
1:B:38[B]:ARG:HH11	1:B:38[B]:ARG:HG3	1.21	1.04
1:B:36[B]:MET:HE3	1:B:44:LEU:HD22	1.07	1.02
1:C:110:GLY:HA2	1:C:304[B]:LYS:HE3	1.47	0.94
1:C:405:ARG:NH1	3:C:2333:HOH:O	2.00	0.94
1:B:87[B]:THR:HG21	3:B:2143:HOH:O	1.68	0.93
1:B:388[A]:LYS:NZ	3:B:2483:HOH:O	1.92	0.91
1:A:228[B]:ILE:HD11	1:A:277:PHE:HZ	1.35	0.90
1:D:36[B]:MET:HA	1:D:36[B]:MET:HE2	1.55	0.88
1:B:36[B]:MET:CE	1:B:44:LEU:HD22	2.01	0.88
1:B:21:PRO:HB3	1:D:319:GLY:HA3	1.60	0.84
1:A:167:LYS:O	1:A:171[B]:GLU:HG2	1.77	0.84
1:B:38[B]:ARG:HG3	1:B:38[B]:ARG:NH1	1.90	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLY:HA2	1:B:304[A]:LYS:HE3	1.62	0.81
1:D:208[A]:LEU:HD22	1:D:248:ILE:HG21	1.63	0.80
1:A:81[B]:GLU:HG3	3:A:2203:HOH:O	1.83	0.79
1:D:208[A]:LEU:HD22	1:D:248:ILE:CG2	2.11	0.79
1:D:208[A]:LEU:HD21	1:D:212:ILE:HD11	1.64	0.78
1:A:228[B]:ILE:CD1	1:A:277:PHE:CZ	2.67	0.77
1:A:451:GLN:NE2	3:A:2714:HOH:O	2.19	0.75
1:C:48:GLU:HA	1:C:48:GLU:OE1	1.86	0.75
1:D:371:ASP:OD2	1:D:388[B]:LYS:HG3	1.87	0.74
1:D:368:GLU:O	1:D:388[A]:LYS:HD2	1.88	0.74
1:B:34[B]:ARG:HG2	1:D:91:THR:HG22	1.70	0.72
1:B:40:GLU:HG2	3:B:2012:HOH:O	1.90	0.70
1:D:208[A]:LEU:CD2	1:D:212:ILE:CD1	2.70	0.69
1:A:228[B]:ILE:HD11	1:A:277:PHE:CE2	2.27	0.69
1:B:319:GLY:HA3	1:D:21:PRO:HB3	1.76	0.68
3:B:2142:HOH:O	1:D:23[A]:THR:HG21	1.94	0.68
1:A:228[B]:ILE:CD1	1:A:277:PHE:CE2	2.77	0.67
1:B:387:ASN:HD22	1:B:390:LYS:H	1.43	0.66
1:B:38[B]:ARG:HH11	1:B:38[B]:ARG:HG2	1.59	0.65
1:B:87[B]:THR:HG23	1:D:21:PRO:HD2	1.78	0.65
1:D:208[A]:LEU:CD2	1:D:212:ILE:HD11	2.26	0.65
1:B:34[B]:ARG:CG	1:D:91:THR:HG22	2.26	0.64
1:B:60:TRP:HE1	1:B:416[B]:ARG:HH21	1.45	0.64
1:B:30:GLN:HE21	1:B:30:GLN:HA	1.64	0.62
1:B:304[A]:LYS:HE2	3:B:2413:HOH:O	1.99	0.61
1:D:356[B]:MET:CE	1:D:360:TRP:HE3	2.12	0.61
1:A:319:GLY:HA3	1:C:21:PRO:HB3	1.83	0.61
1:C:387:ASN:HB3	1:C:392:GLU:HB3	1.82	0.61
1:D:35:VAL:HB	1:D:47[A]:SER:HB2	1.82	0.60
1:D:246:GLU:O	1:D:250[A]:ARG:HG2	2.01	0.60
1:A:315[B]:ASP:OD1	1:C:24:ASP:HB2	2.01	0.60
1:D:208[A]:LEU:HD23	1:D:212:ILE:CD1	2.30	0.60
1:B:36[B]:MET:SD	1:B:37:THR:N	2.75	0.59
1:B:452:THR:O	1:B:456:ARG:HG2	2.03	0.59
1:C:415[A]:MET:HG3	1:C:423:VAL:O	2.03	0.59
1:D:36[B]:MET:SD	1:D:44:LEU:HD22	2.42	0.59
1:A:93:HIS:CE1	1:A:326:PRO:HG3	2.38	0.58
1:C:188[B]:TRP:CZ2	1:C:197:PRO:HD3	2.39	0.58
1:C:61:CYS:O	1:C:292:SER:HA	2.05	0.57
1:C:36[B]:MET:CE	1:C:44:LEU:HD13	2.34	0.57
1:D:208[A]:LEU:HD23	1:D:212:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208[A]:LEU:CD2	1:D:212:ILE:HD12	2.33	0.57
1:B:36[B]:MET:HE2	1:B:44:LEU:HB3	1.87	0.57
1:A:351[B]:ASP:OD1	1:A:432:ARG:NH2	2.39	0.56
1:C:352[B]:ILE:HD11	1:C:435:VAL:HG21	1.88	0.56
1:B:38[B]:ARG:CG	1:B:38[B]:ARG:NH1	2.40	0.56
1:B:94:PRO:O	1:B:98[A]:GLU:HG2	2.06	0.56
1:C:276:HIS:CE1	1:C:376:VAL:HG21	2.41	0.56
1:B:86:ASN:O	1:B:91[B]:THR:HG23	2.05	0.56
1:B:98[B]:GLU:HG2	1:B:333:HIS:CD2	2.41	0.55
1:A:175:LEU:HB3	1:A:176:PRO:HA	1.89	0.55
1:C:244:GLU:CD	1:C:247[A]:ARG:HH21	2.15	0.55
1:C:360:TRP:HH2	1:C:415[B]:MET:CE	2.19	0.55
1:A:304:LYS:HE3	3:A:2542:HOH:O	2.06	0.54
1:C:199:GLU:HA	3:C:2231:HOH:O	2.07	0.54
1:D:344:ILE:O	1:D:348:VAL:HG23	2.06	0.54
1:D:21:PRO:O	1:D:23[A]:THR:HG23	2.07	0.54
1:B:458:LEU:O	1:B:459:ALA:OXT	2.25	0.54
1:D:261:VAL:HG12	1:D:288:LYS:HD2	1.89	0.54
1:D:36[B]:MET:HA	1:D:36[B]:MET:CE	2.34	0.53
1:B:304[A]:LYS:CE	3:B:2413:HOH:O	2.54	0.53
1:B:93:HIS:CE1	1:B:326:PRO:HG3	2.43	0.53
1:D:356[B]:MET:CE	1:D:360:TRP:CE3	2.91	0.53
1:A:228[B]:ILE:HD13	1:A:277:PHE:CE2	2.44	0.53
1:B:116:TYR:HD2	3:B:2190:HOH:O	1.91	0.53
1:D:201:GLY:HA3	1:D:240[A]:THR:HG23	1.91	0.52
1:D:208[A]:LEU:HD22	1:D:248:ILE:HG22	1.87	0.52
1:C:450:GLU:HA	1:C:453:LEU:HD13	1.92	0.51
1:B:250[B]:ARG:HG2	3:B:2366:HOH:O	2.11	0.51
1:D:102:LEU:O	1:D:105:GLU:HG2	2.10	0.51
1:D:167:LYS:O	1:D:171:GLU:HG2	2.11	0.51
1:C:361:ARG:HA	1:C:373:VAL:HG11	1.93	0.51
1:D:160:GLY:HA3	3:D:2082:HOH:O	2.11	0.50
1:B:449:PHE:CE2	1:B:453:LEU:HD12	2.47	0.50
1:D:405:ARG:HA	1:D:408:PHE:HD2	1.76	0.50
1:B:170:HIS:HA	1:B:175:LEU:HB2	1.93	0.50
1:A:21:PRO:HB3	1:C:319:GLY:HA3	1.93	0.50
1:B:369:HIS:HD2	1:B:450:GLU:OE1	1.95	0.50
1:C:453:LEU:O	1:C:454:LYS:C	2.55	0.49
1:A:121:SER:HA	3:A:2310:HOH:O	2.12	0.49
1:A:410[B]:ARG:NH2	1:A:448:GLU:OE2	2.37	0.49
1:D:454:LYS:C	1:D:456[B]:ARG:H	2.21	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:CYS:O	1:A:292:SER:HA	2.13	0.49
1:B:87[B]:THR:HG23	1:D:21:PRO:CD	2.42	0.49
1:A:322:TYR:CD2	1:C:296:PRO:HA	2.48	0.49
1:C:48:GLU:OE1	1:C:48:GLU:CA	2.60	0.49
1:C:405:ARG:HD2	3:C:2332:HOH:O	2.13	0.49
1:C:170:HIS:HA	1:C:175:LEU:HB2	1.95	0.49
1:D:397:PHE:CE1	1:D:420:ASP:HB2	2.48	0.49
1:D:356[B]:MET:HE2	1:D:380:GLN:HG3	1.93	0.48
1:D:454:LYS:C	1:D:456[A]:ARG:H	2.21	0.48
1:B:304[A]:LYS:NZ	3:B:2413:HOH:O	2.42	0.48
1:D:121:SER:HB3	1:D:157:THR:HG23	1.95	0.48
1:D:42:VAL:HG11	1:D:430:MET:HG3	1.94	0.48
1:C:246:GLU:O	1:C:250[A]:ARG:HG2	2.13	0.47
1:A:416[A]:ARG:HB3	1:A:423:VAL:CG2	2.44	0.47
1:B:296:PRO:HA	1:D:322:TYR:CD2	2.50	0.47
1:D:416:ARG:HG3	1:D:417:ALA:N	2.30	0.47
1:D:93:HIS:CE1	1:D:326:PRO:HG3	2.49	0.47
1:B:403[A]:LEU:HD12	3:B:2523:HOH:O	2.14	0.47
1:D:142:GLU:H	1:D:142:GLU:CD	2.22	0.47
1:D:32:GLY:HA2	3:D:2003:HOH:O	2.15	0.47
1:C:352[B]:ILE:HD12	1:C:378:MET:SD	2.55	0.47
1:D:356[B]:MET:HE2	1:D:360:TRP:CE3	2.50	0.47
1:D:355:TYR:CE1	1:D:359:ARG:HG3	2.50	0.46
1:B:250[B]:ARG:HD3	3:B:2372:HOH:O	2.14	0.46
1:B:322:TYR:CD2	1:D:296:PRO:HA	2.49	0.46
1:C:186:PRO:HD2	1:C:229:GLN:OE1	2.15	0.46
1:D:134:TYR:O	1:D:138:GLN:HG2	2.15	0.46
1:D:416:ARG:HD2	3:D:2225:HOH:O	2.16	0.46
1:D:276:HIS:CE1	1:D:376:VAL:HG21	2.50	0.46
1:D:453:LEU:HD23	1:D:458:LEU:HD13	1.96	0.46
1:A:366:ARG:HG2	1:A:366:ARG:HH11	1.81	0.46
1:B:61:CYS:O	1:B:292:SER:HA	2.16	0.46
1:B:352[B]:ILE:HD11	1:B:435:VAL:HG21	1.98	0.46
1:A:82:LEU:HB2	1:C:38:ARG:HA	1.99	0.46
1:C:36[B]:MET:HE2	1:C:44:LEU:HD13	1.98	0.45
1:D:63:ASN:OD1	1:D:267:ARG:NH2	2.49	0.45
1:D:338:ALA:O	1:D:342:GLU:HB2	2.16	0.45
1:C:36[B]:MET:HE3	1:C:44:LEU:HD13	1.98	0.45
1:C:36[B]:MET:HE1	1:C:52:ILE:CD1	2.46	0.45
1:C:453:LEU:HB3	1:C:459:ALA:HB2	1.97	0.45
1:A:234:VAL:O	1:A:234:VAL:HG12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188[B]:TRP:CD1	1:C:197:PRO:HA	2.51	0.45
1:C:389:ALA:N	3:C:2327:HOH:O	2.25	0.45
1:D:134:TYR:HH	1:D:305:ARG:HE	1.61	0.45
1:D:347:ARG:HG3	1:D:351:ASP:HB3	1.98	0.45
1:A:121:SER:HB3	1:A:157:THR:HG23	1.99	0.44
1:D:134:TYR:OH	1:D:305:ARG:NE	2.48	0.44
1:D:196:THR:O	1:D:197:PRO:C	2.60	0.44
1:C:121:SER:HB3	1:C:157:THR:HG23	1.98	0.44
1:D:394:PHE:CG	1:D:400:ILE:HG13	2.52	0.44
1:C:407:ILE:HG12	1:C:410:ARG:HH12	1.83	0.44
1:C:359:ARG:NH1	1:C:362[B]:GLU:OE2	2.51	0.44
1:B:187:TRP:CH2	1:B:393:LEU:HD11	2.52	0.44
1:D:45:TRP:CZ2	1:D:51:LYS:HG3	2.53	0.44
1:D:184:GLU:HB3	1:D:207:TRP:CE3	2.52	0.44
1:C:127:MET:O	1:C:131:VAL:HG23	2.17	0.43
1:B:37:THR:OG1	1:B:38[B]:ARG:CD	2.66	0.43
1:D:388[B]:LYS:HE3	3:D:2215:HOH:O	2.17	0.43
1:C:368:GLU:HB2	3:C:2321:HOH:O	2.18	0.43
1:D:36[B]:MET:HE2	1:D:36[B]:MET:CA	2.28	0.43
1:C:415[A]:MET:HE2	1:C:415[A]:MET:HB2	1.72	0.43
1:C:352[B]:ILE:HD11	1:C:435:VAL:CG2	2.48	0.43
1:B:60:TRP:CD2	1:B:262:ILE:HD13	2.54	0.43
1:C:450:GLU:HA	1:C:453:LEU:CD1	2.49	0.42
1:C:396:ASP:O	1:C:397:PHE:C	2.62	0.42
1:D:456[A]:ARG:HE	1:D:458:LEU:CD1	2.32	0.42
1:C:363:THR:HG23	3:C:2318:HOH:O	2.19	0.42
1:C:244:GLU:OE2	1:C:247[A]:ARG:NH2	2.38	0.42
1:C:416[B]:ARG:HG3	1:C:417:ALA:N	2.32	0.42
1:A:358:LYS:O	1:A:362[A]:GLU:HG3	2.20	0.42
1:B:324:GLY:O	1:B:325:HIS:C	2.61	0.42
1:D:129:ARG:HD3	1:D:318:HIS:ND1	2.33	0.42
1:A:114[B]:VAL:HG23	1:A:116:TYR:CE2	2.55	0.42
1:B:71:PHE:CZ	1:B:335:ASN:HA	2.54	0.42
1:D:208[A]:LEU:HD21	1:D:212:ILE:CD1	2.34	0.42
1:C:127:MET:HE3	1:C:127:MET:HB3	1.96	0.42
1:A:250[A]:ARG:NH2	3:A:2500:HOH:O	2.53	0.42
1:B:114[B]:VAL:HG12	1:B:301:PHE:CD2	2.55	0.42
1:A:227:PRO:C	1:A:228[B]:ILE:HD13	2.45	0.41
1:A:44:LEU:HD11	1:C:85:TYR:CE1	2.55	0.41
1:A:296:PRO:HA	1:C:322:TYR:CD2	2.55	0.41
1:C:387:ASN:ND2	1:C:390:LYS:HE2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:HIS:CD2	1:D:453:LEU:HD13	2.55	0.41
1:A:38[A]:ARG:HA	1:C:82:LEU:HB2	2.02	0.41
1:C:449:PHE:O	1:C:453:LEU:HD12	2.20	0.41
1:D:266:GLY:HA2	1:D:345:VAL:HG13	2.03	0.41
1:C:196:THR:O	1:C:197:PRO:C	2.64	0.41
1:C:36[B]:MET:HE1	1:C:52:ILE:HD13	2.03	0.41
1:B:219[B]:LYS:HB3	1:B:219[B]:LYS:HE3	1.92	0.41
3:B:2157:HOH:O	1:D:13:LEU:HB3	2.21	0.41
1:C:407:ILE:HG22	1:C:408:PHE:N	2.36	0.40
1:C:71:PHE:CZ	1:C:335:ASN:HA	2.56	0.40
1:A:231:ALA:HA	1:A:416[B]:ARG:NH2	2.37	0.40
1:C:394:PHE:CG	1:C:400:ILE:HG13	2.57	0.40
1:C:430:MET:HG3	1:C:434:GLU:HB3	2.02	0.40
1:D:158:ILE:HG23	1:D:175:LEU:CD2	2.50	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	489/459 (106%)	472 (96%)	15 (3%)	2 (0%)	30	12
1	B	486/459 (106%)	470 (97%)	15 (3%)	1 (0%)	43	26
1	C	476/459 (104%)	448 (94%)	23 (5%)	5 (1%)	11	2
1	D	472/459 (103%)	445 (94%)	24 (5%)	3 (1%)	21	7
All	All	1923/1836 (105%)	1835 (95%)	77 (4%)	11 (1%)	21	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	397	PHE
1	C	453	LEU
1	C	454	LYS
1	A	287	ALA
1	C	288	LYS
1	D	287	ALA
1	D	288	LYS
1	A	288	LYS
1	C	287	ALA
1	D	397	PHE

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	400/368 (109%)	398 (100%)	2 (0%)	81	70
1	B	397/368 (108%)	387 (98%)	10 (2%)	42	12
1	C	387/368 (105%)	376 (97%)	11 (3%)	38	9
1	D	384/368 (104%)	373 (97%)	11 (3%)	37	8
All	All	1568/1472 (106%)	1534 (98%)	34 (2%)	53	15

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376[A]	VAL
1	A	376[B]	VAL
1	B	30	GLN
1	B	250[A]	ARG
1	B	250[B]	ARG
1	B	358	LYS
1	B	403[A]	LEU
1	B	403[B]	LEU
1	B	416[A]	ARG
1	B	416[B]	ARG
1	B	444	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	451	GLN
1	C	48	GLU
1	C	280[A]	GLN
1	C	280[B]	GLN
1	C	399	GLU
1	C	405	ARG
1	C	407	ILE
1	C	410	ARG
1	C	415[A]	MET
1	C	415[B]	MET
1	C	453	LEU
1	C	456	ARG
1	D	47[A]	SER
1	D	47[B]	SER
1	D	167	LYS
1	D	171	GLU
1	D	208[A]	LEU
1	D	208[B]	LEU
1	D	315[A]	ASP
1	D	315[B]	ASP
1	D	340	ARG
1	D	358	LYS
1	D	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	B	30	GLN
1	B	50	ASN
1	B	138	GLN
1	B	369	HIS
1	B	387	ASN
1	C	151	ASN
1	C	276	HIS
1	C	369	HIS
1	C	411	ASN
1	D	78	GLN
1	D	151	ASN
1	D	346	GLN
1	D	369	HIS

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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	B	1288	1	15,15,16	2.92	4 (26%)	21,22,23	2.34	5 (23%)
2	PLP	D	1288	1	15,15,16	3.04	3 (20%)	21,22,23	1.79	5 (23%)
2	PLP	C	1288	1	15,15,16	3.18	3 (20%)	21,22,23	2.28	5 (23%)
2	PLP	A	1288	1	15,15,16	2.91	4 (26%)	21,22,23	1.86	6 (28%)

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	PLP	B	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1288	1	-	0/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1288	PLP	C5-C4	8.42	1.50	1.40
2	B	1288	PLP	C5-C4	8.13	1.49	1.40
2	D	1288	PLP	C5-C4	8.03	1.49	1.40
2	A	1288	PLP	C5-C4	7.92	1.49	1.40
2	C	1288	PLP	C3-C2	7.29	1.48	1.41
2	D	1288	PLP	C3-C2	6.98	1.48	1.41
2	B	1288	PLP	C3-C2	6.30	1.47	1.41
2	A	1288	PLP	C3-C2	5.58	1.46	1.41
2	A	1288	PLP	C3-C4	4.52	1.48	1.40
2	C	1288	PLP	C3-C4	4.51	1.48	1.40
2	D	1288	PLP	C3-C4	3.88	1.47	1.40
2	B	1288	PLP	C3-C4	3.44	1.46	1.40
2	A	1288	PLP	C2-N1	2.02	1.37	1.33
2	B	1288	PLP	P-O3P	-2.01	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1288	PLP	C4A-C4-C5	7.84	129.02	120.94
2	C	1288	PLP	C4A-C4-C5	7.64	128.82	120.94
2	D	1288	PLP	C4A-C4-C5	5.01	126.11	120.94
2	A	1288	PLP	C4A-C4-C5	4.58	125.66	120.94
2	B	1288	PLP	C3-C4-C5	-4.06	113.72	118.59
2	C	1288	PLP	C3-C4-C5	-4.04	113.74	118.59
2	A	1288	PLP	C3-C2-N1	-3.48	116.57	120.96
2	B	1288	PLP	C6-C5-C4	3.32	120.82	118.10
2	A	1288	PLP	C6-N1-C2	3.00	124.64	119.20
2	A	1288	PLP	C3-C4-C5	-2.78	115.25	118.59
2	B	1288	PLP	C2A-C2-C3	-2.76	117.57	120.80
2	D	1288	PLP	C3-C4-C5	-2.67	115.39	118.59
2	D	1288	PLP	C2A-C2-C3	-2.47	117.90	120.80
2	C	1288	PLP	C6-C5-C4	2.41	120.07	118.10
2	D	1288	PLP	C2A-C2-N1	2.38	122.13	117.64
2	C	1288	PLP	O4P-C5A-C5	2.38	113.81	109.36
2	D	1288	PLP	C6-C5-C4	2.32	120.00	118.10
2	A	1288	PLP	C5A-C5-C6	-2.20	115.78	119.36
2	A	1288	PLP	C2A-C2-N1	2.15	121.69	117.64
2	B	1288	PLP	C4A-C4-C3	-2.07	117.07	120.52
2	C	1288	PLP	O3-C3-C2	2.01	121.75	117.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	455/459 (99%)	0.07	4 (0%) 81 86	6, 15, 26, 42	36 (7%)
1	B	455/459 (99%)	0.52	38 (8%) 17 25	10, 20, 43, 73	33 (7%)
1	C	455/459 (99%)	1.03	74 (16%) 4 8	10, 26, 61, 109	23 (5%)
1	D	454/459 (98%)	1.53	120 (26%) 1 2	15, 33, 63, 93	20 (4%)
All	All	1819/1836 (99%)	0.78	236 (12%) 7 12	6, 23, 54, 109	112 (6%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	ALA	6.6
1	D	409	PHE	6.0
1	C	367	PHE	5.2
1	C	459	ALA	4.7
1	C	394	PHE	4.6
1	D	35	VAL	4.5
1	C	458	LEU	4.4
1	D	188	TRP	4.4
1	D	348	VAL	4.4
1	D	449	PHE	4.3
1	D	385	VAL	4.3
1	B	459	ALA	4.3
1	D	355	TYR	4.1
1	D	10	TRP	4.1
1	D	458	LEU	4.1
1	D	13	LEU	4.0
1	D	433	ALA	4.0
1	C	440	ALA	4.0
1	C	449	PHE	3.8
1	C	455	ALA	3.8
1	D	360	TRP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	458	LEU	3.7
1	C	408	PHE	3.7
1	D	435	VAL	3.7
1	D	457	GLY	3.6
1	B	15	ALA	3.6
1	C	189	TYR	3.6
1	C	200	PHE	3.6
1	C	33	ALA	3.6
1	D	455	ALA	3.5
1	C	188[A]	TRP	3.5
1	D	352	ILE	3.5
1	D	453	LEU	3.5
1	D	408	PHE	3.4
1	C	453	LEU	3.4
1	B	88	PHE	3.3
1	B	25	THR	3.3
1	C	442	ALA	3.3
1	D	363	THR	3.2
1	C	385	VAL	3.2
1	D	446	LEU	3.2
1	B	91[A]	THR	3.2
1	C	196	THR	3.2
1	D	407	ILE	3.2
1	D	382	PHE	3.2
1	C	10	TRP	3.2
1	C	369	HIS	3.2
1	C	446	LEU	3.1
1	D	248	ILE	3.1
1	D	271	TRP	3.1
1	C	373	VAL	3.1
1	D	345	VAL	3.1
1	C	354	PRO	3.1
1	C	457	GLY	3.1
1	D	45	TRP	3.1
1	D	106	VAL	3.1
1	C	241	TYR	3.1
1	D	23[A]	THR	3.1
1	B	89	PHE	3.1
1	D	364	PHE	3.1
1	D	71	PHE	3.0
1	D	200	PHE	3.0
1	B	33	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	381	ALA	3.0
1	C	370	VAL	3.0
1	C	409	PHE	3.0
1	C	389	ALA	3.0
1	D	96	VAL	3.0
1	C	411	ASN	2.9
1	C	441	VAL	2.9
1	B	13	LEU	2.9
1	D	393	LEU	2.9
1	D	403	LEU	2.9
1	D	89	PHE	2.9
1	D	377	GLY	2.9
1	C	407	ILE	2.9
1	D	431	THR	2.9
1	D	103	LEU	2.9
1	D	343	GLY	2.9
1	D	316	PHE	2.8
1	C	368	GLU	2.8
1	D	49	GLY	2.8
1	D	16	ALA	2.8
1	C	53[A]	ILE	2.8
1	D	235	ILE	2.8
1	D	344	ILE	2.8
1	D	452	THR	2.8
1	C	360	TRP	2.8
1	C	445	CYS	2.8
1	D	439	LEU	2.8
1	D	97	VAL	2.8
1	B	21	PRO	2.8
1	B	83	PRO	2.8
1	C	452	THR	2.8
1	B	35	VAL	2.7
1	D	441	VAL	2.7
1	D	107	THR	2.7
1	C	245	ILE	2.7
1	D	322	TYR	2.7
1	B	403[A]	LEU	2.7
1	B	97	VAL	2.7
1	C	413	LEU	2.7
1	D	373	VAL	2.7
1	D	196	THR	2.7
1	C	195	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.6
1	C	400	ILE	2.6
1	C	433	ALA	2.6
1	D	31	ALA	2.6
1	D	338	ALA	2.6
1	B	14	ASP	2.6
1	B	28	LEU	2.6
1	D	86	ASN	2.6
1	B	32	GLY	2.6
1	D	18	HIS	2.6
1	C	6	THR	2.6
1	D	402	THR	2.6
1	D	43	TYR	2.6
1	D	197	PRO	2.6
1	D	354	PRO	2.6
1	B	45	TRP	2.5
1	C	45	TRP	2.5
1	C	402	THR	2.5
1	C	43	TYR	2.5
1	D	277	PHE	2.5
1	D	401	GLY	2.5
1	D	370	VAL	2.5
1	D	52	ILE	2.5
1	D	422	ILE	2.5
1	B	322	TYR	2.5
1	D	67	GLY	2.5
1	D	353	GLY	2.5
1	D	62	VAL	2.5
1	D	91	THR	2.5
1	C	204	ALA	2.5
1	C	248	ILE	2.5
1	D	289	GLY	2.5
1	C	197	PRO	2.5
1	D	367	PHE	2.5
1	D	417	ALA	2.4
1	D	278	GLY	2.4
1	D	350	ASP	2.4
1	B	26	ALA	2.4
1	B	455	ALA	2.4
1	C	386	LYS	2.4
1	C	355	TYR	2.4
1	B	6	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	87[A]	THR	2.4
1	B	22	PHE	2.4
1	D	440	ALA	2.4
1	D	376	VAL	2.4
1	B	24	ASP	2.3
1	C	254	VAL	2.3
1	D	378	MET	2.3
1	D	25	THR	2.3
1	C	454	LYS	2.3
1	D	187	TRP	2.3
1	C	387	ASN	2.3
1	D	206	ARG	2.3
1	B	96	VAL	2.3
1	C	203	VAL	2.3
1	C	236	VAL	2.3
1	D	32	GLY	2.3
1	D	17	HIS	2.3
1	D	414	ILE	2.3
1	B	50	ASN	2.2
1	D	50	ASN	2.2
1	D	412	ASN	2.2
1	A	84	PHE	2.2
1	B	7	THR	2.2
1	D	88	PHE	2.2
1	C	398	GLY	2.2
1	D	413	LEU	2.2
1	D	53	ILE	2.2
1	D	26	ALA	2.2
1	B	23	THR	2.2
1	B	93	HIS	2.2
1	C	443	GLU	2.2
1	D	349	LYS	2.2
1	D	65	GLY	2.2
1	D	266	GLY	2.2
1	C	205	ALA	2.2
1	C	388	LYS	2.2
1	D	93	HIS	2.2
1	C	41	GLY	2.2
1	C	431	THR	2.2
1	D	410	ARG	2.2
1	B	409	PHE	2.2
1	D	236	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	2.1
1	D	28	LEU	2.1
1	C	238	PRO	2.1
1	D	33	ALA	2.1
1	B	49	GLY	2.1
1	B	92	THR	2.1
1	C	404	CYS	2.1
1	D	358	LYS	2.1
1	D	22	PHE	2.1
1	D	279	PHE	2.1
1	C	42	VAL	2.1
1	B	5	ARG	2.1
1	B	323	SER	2.1
1	C	192	GLY	2.1
1	D	365	SER	2.1
1	C	403	LEU	2.1
1	D	12	GLU	2.1
1	B	36[A]	MET	2.1
1	C	410	ARG	2.1
1	D	366	ARG	2.1
1	D	42	VAL	2.1
1	D	108	PRO	2.1
1	D	436	ASP	2.1
1	A	459	ALA	2.1
1	D	7	THR	2.1
1	D	381	ALA	2.1
1	D	418	CYS	2.1
1	D	445	CYS	2.1
1	A	174	ASP	2.1
1	C	49	GLY	2.1
1	D	46	ASP	2.1
1	C	364	PHE	2.0
1	C	382	PHE	2.0
1	D	92	THR	2.0
1	C	202	VAL	2.0
1	C	376	VAL	2.0
1	D	336	VAL	2.0
1	D	205	ALA	2.0
1	C	391	ARG	2.0
1	C	447	GLU	2.0
1	D	387	ASN	2.0
1	D	237	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	10	TRP	2.0
1	D	362	GLU	2.0
1	C	31	ALA	2.0
1	B	102	LEU	2.0
1	D	404	CYS	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 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
2	PLP	D	1288	15/16	0.94	0.08	21,25,31,33	0
2	PLP	B	1288	15/16	0.95	0.07	14,20,24,32	0
2	PLP	C	1288	15/16	0.96	0.07	17,18,27,34	0
2	PLP	A	1288	15/16	0.97	0.05	9,10,13,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.