



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:53 AM UTC

PDB ID : 8OJZ / pdb_00008ojz
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase 1 (PPC1) G678S mutant
Authors : Loris, R.; Haesaerts, S.; Larsen, P.B.
Deposited on : 2023-03-25
Resolution : 3.25 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

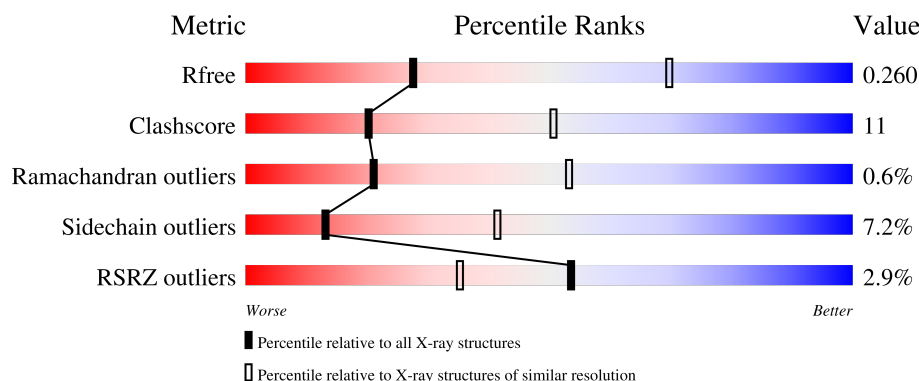
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 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	974	
1	B	974	

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	PO4	A	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14457 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.

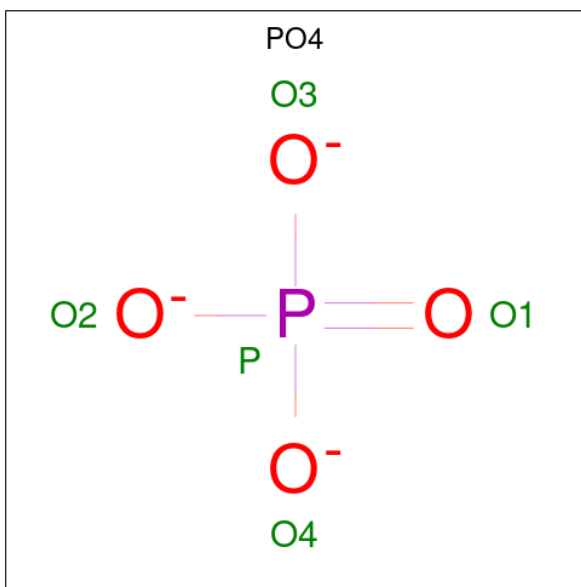
- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	3	0
			7268	4615	1273	1351	29			
1	B	890	Total	C	N	O	S	0	0	0
			7144	4534	1245	1336	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
A	678	SER	GLY	engineered mutation	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0
B	678	SER	GLY	engineered mutation	UNP Q9MAH0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

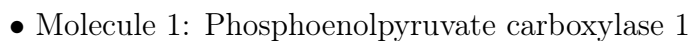


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		

- Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.27Å 160.28Å 141.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.25 49.32 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.32-3.25) 99.5 (49.32-3.25)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.220 , 0.261 0.225 , 0.260	Depositor DCC
R_{free} test set	2322 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14457	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: PO4

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	0.33	0/7435	0.55	0/10068
1	B	0.20	0/7297	0.41	0/9879
All	All	0.27	0/14732	0.49	0/19947

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

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	7268	0	7202	174	0
1	B	7144	0	7086	151	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
3	A	35	0	0	2	0
All	All	14457	0	14288	324	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 11.

All (324) 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:173:HIS:ND1	1:A:669:GLN:OE1	2.00	0.94
1:B:173:HIS:ND1	1:B:669:GLN:OE1	2.10	0.85
1:B:404:ASN:HB2	1:B:407:GLN:HB2	1.58	0.85
1:A:618:GLU:OE1	1:A:710:ARG:NH2	2.13	0.81
1:B:172:ALA:HB2	1:B:285:MET:HG3	1.64	0.80
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.64	0.80
1:B:332:ASN:HD21	1:B:418:SER:HA	1.48	0.78
1:B:306:LEU:HD22	1:B:389:LEU:HD11	1.68	0.76
1:A:332:ASN:HD21	1:A:418:SER:HA	1.50	0.75
1:A:158:PHE:HB2	1:A:268:ILE:HD13	1.69	0.74
1:A:528:TYR:HB2	1:A:555:LEU:HD13	1.69	0.73
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.71	0.72
1:B:460:ASP:OD1	1:B:475:ARG:NH1	2.22	0.72
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.71	0.72
1:B:237:MET:HE3	1:B:303:VAL:HB	1.73	0.71
1:A:345:ASN:OD1	1:A:345:ASN:N	2.22	0.71
1:B:345:ASN:N	1:B:345:ASN:OD1	2.22	0.71
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.71	0.71
1:A:332:ASN:ND2	1:A:418:SER:HA	2.07	0.69
1:B:702:PRO:HB3	1:B:816:PRO:HG2	1.76	0.68
1:A:723:GLU:HG2	1:A:789:GLY:HA2	1.74	0.68
1:B:158:PHE:HB2	1:B:268:ILE:HD13	1.76	0.68
1:B:175:THR:HG23	1:B:671:GLU:H	1.59	0.68
1:A:237:MET:HE3	1:A:303:VAL:HB	1.75	0.67
1:A:326:MET:HE1	1:A:419:LEU:HD11	1.76	0.67
1:A:844:LEU:HD22	1:A:909:ARG:HH21	1.58	0.67
1:B:169:VAL:HB	1:B:282:SER:HB2	1.77	0.67
1:A:772:PRO:HA	1:A:775:PHE:HB3	1.76	0.67
1:A:306:LEU:O	1:A:310:MET:HG3	1.94	0.67
1:A:517:ILE:HD13	1:A:555:LEU:HD21	1.78	0.66
1:A:497:PHE:HD1	1:A:497:PHE:H	1.44	0.66
1:A:716:MET:HG3	1:A:793:ALA:HB1	1.78	0.66
1:A:450:ASP:OD2	1:A:665:ARG:NH2	2.29	0.65
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.78	0.65
1:B:772:PRO:HA	1:B:775:PHE:HB3	1.79	0.65
1:A:755:ARG:HD3	1:A:769:ARG:NH2	2.12	0.64
1:A:34:ASP:O	1:A:38:LEU:HB2	1.97	0.64
1:A:175:THR:HG23	1:A:671:GLU:H	1.60	0.64
1:B:384:ARG:HD2	1:B:396:VAL:HB	1.80	0.63
1:B:638:GLY:HA2	1:B:669:GLN:HG3	1.79	0.63
1:A:641:VAL:HG21	1:A:828:VAL:HG21	1.78	0.63
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:GLU:HG3	1:A:952:LEU:HD21	1.81	0.62
1:B:843:LEU:HD22	1:B:906:LYS:HD2	1.82	0.62
1:B:253:PRO:O	1:B:257:ARG:HG3	1.99	0.62
1:B:656:PRO:HG2	1:B:659:THR:HG21	1.81	0.62
1:A:908:ILE:HD12	1:A:944:TYR:CD2	2.35	0.61
1:B:593:VAL:HG12	1:B:631:LEU:HD11	1.82	0.61
1:B:888:ARG:O	1:B:890:ARG:N	2.34	0.61
1:A:315:TYR:HB3	1:A:378:LEU:HD21	1.83	0.61
1:A:106:ASN:OD1	1:A:890:ARG:NH2	2.34	0.60
1:A:908:ILE:HD11	1:A:948:LEU:HB3	1.82	0.60
1:A:228:ARG:HH12	1:A:938:LEU:HB3	1.67	0.59
1:A:449:LEU:O	1:A:526:GLY:N	2.27	0.59
1:A:884:LYS:HA	1:A:887:LEU:HD23	1.83	0.59
1:B:908:ILE:HD11	1:B:948:LEU:HB3	1.84	0.59
1:A:252:VAL:HG13	1:A:279:ILE:HD11	1.84	0.59
1:A:318:GLN:HB3	1:A:435:PHE:HE1	1.66	0.58
1:B:332:ASN:ND2	1:B:418:SER:HA	2.16	0.58
1:A:739:ARG:NH1	1:A:744:GLU:OE1	2.37	0.57
1:A:593:VAL:HG12	1:A:631:LEU:HD11	1.86	0.57
1:B:181:SER:OG	2:B:1001:PO4:O1	2.17	0.57
1:B:610:ALA:HA	1:B:613:LEU:HD12	1.86	0.57
1:A:416:TYR:CD2	1:A:428:ALA:HB1	2.39	0.57
1:A:243:TYR:OH	1:A:674:GLU:HG2	2.04	0.57
1:B:318:GLN:HB3	1:B:435:PHE:HE1	1.70	0.57
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.20	0.56
1:A:201:ILE:H	1:A:201:ILE:HD13	1.71	0.56
1:A:416:TYR:OH	1:A:429:ASP:OD1	2.17	0.56
1:B:306:LEU:O	1:B:310:MET:HG3	2.05	0.56
1:B:528:TYR:HB2	1:B:555:LEU:HD13	1.88	0.56
1:A:638:GLY:HA2	1:A:669:GLN:CG	2.34	0.56
1:B:611:TRP:CZ2	1:B:615:LYS:HE3	2.40	0.56
1:A:37:LEU:HD21	1:A:193:LEU:HD21	1.88	0.56
1:A:237:MET:O	1:A:241:MET:HG2	2.06	0.55
1:B:844:LEU:HD22	1:B:909:ARG:HH21	1.72	0.55
1:A:237:MET:HG2	1:A:303:VAL:HG12	1.87	0.55
1:A:794:ILE:O	1:A:798:ILE:HG12	2.07	0.54
1:A:262:ALA:O	1:A:266:ILE:HG12	2.07	0.54
1:B:478:SER:H	1:B:481:ARG:NH1	2.04	0.54
1:A:167:ASP:HB3	1:A:665:ARG:HG3	1.88	0.54
1:A:618:GLU:CD	1:A:710:ARG:HH22	2.16	0.54
1:A:915:VAL:N	1:A:943:GLU:O	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:VAL:HG23	1:A:729:PHE:CD2	2.43	0.54
1:B:477:TRP:CG	1:B:481:ARG:HD2	2.43	0.54
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.90	0.53
1:A:406:GLU:HB3	1:A:409:LEU:HD12	1.89	0.53
1:B:315:TYR:HB3	1:B:378:LEU:HD21	1.90	0.53
1:A:602:LYS:NZ	1:A:768:LEU:O	2.33	0.53
1:B:621:VAL:HG21	1:B:659:THR:HG22	1.91	0.53
1:A:582:TRP:O	1:A:586:ARG:HD3	2.08	0.53
1:B:824:LEU:O	1:B:828:VAL:HG23	2.08	0.53
1:B:582:TRP:O	1:B:586:ARG:HD3	2.09	0.53
1:A:302:ASP:O	1:A:306:LEU:HB2	2.09	0.52
1:B:513:THR:O	1:B:517:ILE:HG13	2.10	0.52
1:B:728:VAL:HG23	1:B:729:PHE:CD2	2.45	0.52
1:A:656:PRO:HG2	1:A:659:THR:HG21	1.92	0.52
1:B:237:MET:O	1:B:241:MET:HG2	2.10	0.52
1:A:527:ALA:HB2	1:A:556:ARG:CZ	2.39	0.52
1:B:716:MET:SD	1:B:797:VAL:HG21	2.49	0.52
1:A:169:VAL:HB	1:A:282:SER:HB2	1.92	0.52
1:B:497:PHE:HD1	1:B:497:PHE:H	1.58	0.52
1:A:404:ASN:HB2	1:A:407:GLN:HB2	1.92	0.52
1:B:308:ARG:HG3	1:B:445:SER:HB3	1.91	0.52
1:B:454:GLU:HA	1:B:531:SER:HB2	1.91	0.51
1:A:165:THR:HG22	1:A:663:SER:HA	1.91	0.51
1:A:716:MET:CG	1:A:793:ALA:HB1	2.41	0.51
1:A:723:GLU:O	1:A:726:SER:OG	2.28	0.51
1:A:249:TRP:HE1	1:A:318:GLN:HE22	1.59	0.51
1:A:733:ARG:CZ	1:A:849:LEU:HD13	2.40	0.51
1:B:638:GLY:HA2	1:B:669:GLN:CG	2.39	0.51
1:B:724:TYR:CD1	1:B:788:LEU:HD23	2.46	0.51
1:A:641:VAL:HG21	1:A:828:VAL:CG2	2.40	0.51
1:A:786:VAL:HG11	1:A:828:VAL:HG21	1.93	0.51
1:B:201:ILE:HD13	1:B:201:ILE:H	1.75	0.51
1:B:642:GLY:HA3	1:B:774:ILE:HD12	1.92	0.51
1:B:794:ILE:O	1:B:798:ILE:HG12	2.10	0.51
1:B:887:LEU:HD23	1:B:887:LEU:H	1.76	0.51
1:A:83:LEU:HD12	1:A:899:VAL:HG12	1.92	0.51
1:A:49:HIS:HB3	1:A:53:LEU:HD23	1.92	0.50
1:A:399:GLU:CD	1:A:399:GLU:H	2.18	0.50
1:B:33:TYR:HE1	1:B:36:LEU:HD22	1.75	0.50
1:A:846:SER:HB3	3:A:1123:HOH:O	2.12	0.50
1:B:723:GLU:HG2	1:B:789:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD13	1:B:695:LEU:HD22	1.92	0.50
1:B:641:VAL:HG21	1:B:828:VAL:HG21	1.93	0.50
1:A:607:LEU:HB2	1:A:790:PHE:CE1	2.47	0.50
1:A:245:HIS:HA	1:A:314:MET:HE1	1.93	0.50
1:B:37:LEU:HD11	1:B:108:ALA:HB2	1.94	0.49
1:B:672:VAL:O	1:B:676:SER:OG	2.30	0.49
1:A:244:PHE:C	1:A:246:GLU:H	2.20	0.49
1:B:716:MET:HG3	1:B:793:ALA:HB1	1.93	0.49
1:A:843:LEU:HD22	1:A:906:LYS:HD2	1.94	0.49
1:B:861:GLU:HG3	1:B:865:LYS:HE3	1.95	0.49
1:B:60:LEU:HD21	1:B:83:LEU:HD21	1.94	0.49
1:A:202:THR:O	1:A:205:ASP:N	2.45	0.49
1:A:326:MET:HE1	1:A:419:LEU:CD1	2.43	0.49
1:B:501:LEU:O	1:B:503:LYS:HG3	2.13	0.49
1:A:58:GLN:O	1:A:62:GLU:HG3	2.13	0.49
1:B:244:PHE:C	1:B:246:GLU:H	2.20	0.49
1:A:244:PHE:HA	1:A:248:ILE:HB	1.94	0.49
1:B:60:LEU:HG	1:B:79:LEU:HD21	1.94	0.49
1:A:343:HIS:HA	1:A:346:SER:HB2	1.94	0.48
1:A:558:VAL:HG23	1:A:593:VAL:HA	1.94	0.48
1:A:112:GLN:O	1:A:116:ARG:HB2	2.14	0.48
1:A:150:LEU:HD11	1:A:700:ARG:HB2	1.96	0.48
1:A:336:ARG:NH2	1:A:366:PRO:HG3	2.29	0.48
1:B:240:GLY:HA3	1:B:285:MET:CE	2.44	0.47
1:A:40:ARG:O	1:A:44:ILE:HG13	2.13	0.47
1:A:457:ARG:NE	1:A:506:GLU:HB3	2.29	0.47
1:B:791:GLY:HA2	1:B:866:LEU:HD12	1.96	0.47
1:A:172:ALA:HB2	1:A:285:MET:HG3	1.95	0.47
1:A:452:ARG:HG3	1:A:529:ILE:HB	1.96	0.47
1:A:460:ASP:OD1	1:A:475:ARG:NH1	2.46	0.47
1:A:174:PRO:O	1:A:747:TYR:OH	2.33	0.47
1:A:497:PHE:N	1:A:497:PHE:CD1	2.83	0.47
1:B:594:MET:HA	1:B:634:PHE:HB3	1.96	0.47
1:B:240:GLY:HA3	1:B:285:MET:HE3	1.97	0.47
1:B:563:LYS:NZ	1:B:766:GLU:OE2	2.48	0.47
1:B:618:GLU:OE1	1:B:710:ARG:NH2	2.48	0.47
1:B:952:LEU:O	1:B:955:THR:OG1	2.24	0.47
1:A:294:ARG:HD3	1:A:754:SER:O	2.14	0.47
1:B:150:LEU:HD11	1:B:700:ARG:HD3	1.97	0.47
1:A:298:GLU:OE1	1:A:301[A]:ARG:NH1	2.48	0.47
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:O	1:B:116:ARG:HB2	2.15	0.47
1:A:607:LEU:HB2	1:A:790:PHE:CZ	2.50	0.46
1:A:237:MET:HE2	1:A:237:MET:HB2	1.81	0.46
1:B:587:ILE:HD13	1:B:587:ILE:HA	1.76	0.46
1:A:724:TYR:CE2	1:A:728:VAL:HG21	2.50	0.46
1:A:844:LEU:HD13	1:A:909:ARG:NH2	2.31	0.46
1:A:621:VAL:HG21	1:A:659:THR:HG22	1.98	0.46
1:A:90:ASP:O	1:A:94:ILE:HG12	2.16	0.46
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.79	0.46
1:B:497:PHE:HE1	1:B:548:GLU:HG3	1.81	0.46
1:A:218:GLN:O	1:A:222:ARG:HB2	2.16	0.46
1:B:90:ASP:O	1:B:94:ILE:HG12	2.15	0.46
1:B:256:LEU:HB3	1:B:437:ARG:CZ	2.46	0.46
1:B:890:ARG:O	1:B:894:ILE:HG13	2.15	0.46
1:A:87:ASP:HB3	1:A:88:PRO:HD2	1.97	0.46
1:B:78:GLU:O	1:B:81:SER:OG	2.34	0.46
1:B:336:ARG:NH2	1:B:363:THR:O	2.48	0.46
1:B:611:TRP:CE2	1:B:615:LYS:HE3	2.51	0.46
1:B:739:ARG:HB3	1:B:745:LEU:HD11	1.97	0.46
1:A:501:LEU:O	1:A:503:LYS:HG3	2.15	0.46
1:B:410:GLU:HB3	1:B:411:PRO:HD3	1.97	0.45
1:B:506:GLU:O	1:B:510:VAL:HG12	2.16	0.45
1:B:558:VAL:HG23	1:B:593:VAL:HA	1.98	0.45
1:A:308:ARG:NH2	1:A:523:ASP:OD1	2.49	0.45
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.76	0.45
1:A:442:PHE:HB3	1:A:446:LEU:HD23	1.98	0.45
1:A:848:GLU:O	1:A:851:PRO:HD2	2.17	0.45
1:B:746:GLU:HG3	1:B:952:LEU:HD21	1.98	0.45
1:A:234:GLN:NE2	1:A:299:VAL:HG22	2.31	0.45
1:A:240:GLY:HA3	1:A:285:MET:HE3	1.99	0.45
1:A:326:MET:HG3	1:A:371:LEU:HD11	1.98	0.45
1:A:416:TYR:CE2	1:A:428:ALA:HB1	2.52	0.45
1:A:918:ARG:NE	3:A:1101:HOH:O	2.19	0.45
1:A:945:ALA:HB1	1:A:946:PRO:HD2	1.99	0.45
1:A:305:LEU:HD13	1:A:305:LEU:HA	1.83	0.45
1:A:606[A]:ARG:HA	1:A:606[A]:ARG:HD2	1.88	0.45
1:B:405:LEU:HD12	1:B:405:LEU:H	1.82	0.45
1:B:450:ASP:OD2	1:B:665:ARG:NH2	2.50	0.45
1:B:552:LYS:HG3	1:B:553:GLN:OE1	2.17	0.45
1:B:724:TYR:O	1:B:728:VAL:HG22	2.17	0.45
1:A:301[B]:ARG:HA	1:A:520:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:O	1:A:84:THR:HG23	2.17	0.44
1:A:301[A]:ARG:HA	1:A:520:LEU:HD11	1.97	0.44
1:B:61:TYR:HE1	1:B:889:LEU:HD11	1.82	0.44
1:B:139:LEU:N	1:B:688:GLN:OE1	2.50	0.44
1:B:712:LEU:HD11	1:B:797:VAL:HG13	1.99	0.44
1:A:180:ARG:N	2:A:1001:PO4:O4	2.50	0.44
1:A:480:GLU:H	1:A:480:GLU:HG2	1.47	0.44
1:A:506:GLU:O	1:A:510:VAL:HG12	2.18	0.44
1:B:89:GLY:O	1:B:93:VAL:HG23	2.18	0.44
1:A:338:ARG:O	1:A:342:VAL:HG23	2.17	0.44
1:A:490:LEU:HB3	1:A:582:TRP:CZ2	2.52	0.44
1:A:495:PRO:O	1:B:494:ARG:NE	2.46	0.44
1:A:733:ARG:NH1	1:A:849:LEU:HD13	2.32	0.44
1:A:953:ILE:HA	1:A:956:MET:HE3	2.00	0.44
1:A:755:ARG:HD3	1:A:769:ARG:CZ	2.48	0.44
1:B:457:ARG:NE	1:B:506:GLU:HB3	2.33	0.44
1:B:615:LYS:NZ	1:B:714:ASP:OD1	2.34	0.44
1:B:52:ASP:OD1	1:B:52:ASP:N	2.51	0.44
1:B:416:TYR:CD2	1:B:428:ALA:HB1	2.53	0.43
1:A:463:ASP:HB2	1:A:475:ARG:HG3	1.99	0.43
1:B:587:ILE:HD12	1:B:590:LYS:O	2.18	0.43
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.80	0.43
1:A:252:VAL:HG11	1:A:441:THR:HG21	1.99	0.43
1:A:252:VAL:HB	1:A:253:PRO:HD3	2.01	0.43
1:B:157:ILE:O	1:B:161:LEU:HB2	2.18	0.43
1:B:202:THR:O	1:B:205:ASP:N	2.50	0.43
1:B:350:ALA:HB1	1:B:352:LYS:HG3	2.00	0.43
1:A:583:TYR:CZ	1:A:587:ILE:HG12	2.54	0.43
1:B:66:GLU:HB2	1:B:75:LYS:HE2	2.01	0.43
1:B:168:LEU:O	1:B:281:PHE:HA	2.18	0.43
1:B:463:ASP:HB2	1:B:475:ARG:HG3	2.00	0.43
1:A:283:SER:O	1:A:449:LEU:HD12	2.17	0.43
1:B:477:TRP:HA	1:B:481:ARG:NH1	2.34	0.43
1:B:590:LYS:HG2	1:B:630:LYS:HE2	2.00	0.43
1:B:821:THR:O	1:B:825:ILE:HG12	2.17	0.43
1:B:167:ASP:HB3	1:B:665:ARG:HG3	2.01	0.43
1:B:169:VAL:HA	1:B:282:SER:O	2.19	0.43
1:B:365:GLU:H	1:B:365:GLU:HG2	1.71	0.43
1:B:723:GLU:O	1:B:726:SER:OG	2.35	0.43
1:A:454:GLU:HA	1:A:531:SER:HB2	2.00	0.42
1:B:157:ILE:HG23	1:B:695:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LEU:HB3	1:B:497:PHE:H	1.68	0.42
1:A:724:TYR:HD1	1:A:788:LEU:HB3	1.84	0.42
1:A:834:PRO:HG3	1:A:860:PHE:CE1	2.55	0.42
1:A:857:ARG:O	1:A:860:PHE:HB3	2.20	0.42
1:B:244:PHE:HA	1:B:248:ILE:HB	2.00	0.42
1:B:451:ILE:HG13	1:B:517:ILE:HD11	2.01	0.42
1:B:510:VAL:O	1:B:513:THR:OG1	2.29	0.42
1:B:723:GLU:OE1	1:B:792:SER:OG	2.27	0.42
1:B:528:TYR:HB2	1:B:555:LEU:CD1	2.49	0.42
1:A:234:GLN:HE22	1:A:299:VAL:HG22	1.83	0.42
1:B:603:ASP:OD1	1:B:603:ASP:N	2.43	0.42
1:B:786:VAL:HG11	1:B:828:VAL:HG11	2.01	0.42
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.84	0.42
1:B:497:PHE:CD1	1:B:497:PHE:N	2.87	0.42
1:B:733:ARG:NH2	1:B:736:GLU:OE2	2.52	0.42
1:A:139:LEU:HD11	1:A:259:VAL:HG22	2.01	0.42
1:B:294:ARG:HD3	1:B:754:SER:O	2.19	0.42
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.70	0.42
1:A:716:MET:SD	1:A:797:VAL:HG21	2.58	0.42
1:B:562:GLU:HG2	1:B:599:ASP:HB2	2.02	0.42
1:A:86:LEU:HD13	1:A:94:ILE:HG13	2.01	0.42
1:A:179:ARG:HB2	2:A:1001:PO4:O4	2.19	0.42
1:A:463:ASP:CG	1:A:475:ARG:HG3	2.45	0.42
1:A:497:PHE:HE1	1:A:548:GLU:HG3	1.85	0.42
1:B:96:LYS:HE2	1:B:225:GLU:OE2	2.20	0.42
1:A:169:VAL:HA	1:A:282:SER:O	2.19	0.42
1:A:768:LEU:HD13	1:A:769:ARG:O	2.20	0.42
1:B:273:PRO:HB2	1:B:276:ALA:HB2	2.01	0.42
1:B:302:ASP:O	1:B:306:LEU:HB2	2.20	0.42
1:A:496:LEU:HB3	1:A:497:PHE:H	1.64	0.42
1:B:48:LEU:HD22	1:B:222:ARG:NH1	2.35	0.41
1:A:611:TRP:CZ2	1:A:615:LYS:HD3	2.55	0.41
1:B:153:SER:OG	1:B:156:GLU:HG3	2.20	0.41
1:B:406:GLU:HA	1:B:409:LEU:HB2	2.02	0.41
1:A:76:LEU:HB3	1:A:839:LEU:HD22	2.02	0.41
1:A:242:SER:HA	1:A:245:HIS:NE2	2.36	0.41
1:B:591:GLN:NE2	1:B:592:GLU:O	2.48	0.41
1:A:462:LEU:O	1:A:466:THR:HG23	2.20	0.41
1:A:784:LEU:HB3	1:A:785:PRO:HD3	2.02	0.41
1:B:86:LEU:HD13	1:B:94:ILE:HG13	2.03	0.41
1:B:289:ARG:HG2	1:B:452:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD21	1:A:83:LEU:HD21	2.02	0.41
1:A:402:PHE:CZ	1:A:408:PHE:HA	2.56	0.41
1:A:724:TYR:CD1	1:A:788:LEU:HD23	2.55	0.41
1:B:614:TYR:CZ	1:B:656:PRO:HB3	2.56	0.41
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.90	0.41
1:A:490:LEU:HD13	1:A:582:TRP:CZ3	2.56	0.41
1:B:245:HIS:H	1:B:245:HIS:CD2	2.38	0.41
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.90	0.41
1:B:724:TYR:CE2	1:B:728:VAL:HG21	2.56	0.41
1:A:52:ASP:OD1	1:A:52:ASP:N	2.54	0.41
1:A:118:ARG:C	1:A:120:LYS:H	2.29	0.41
1:A:274:TYR:OH	1:A:413:GLU:OE2	2.35	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.91	0.41
1:A:530:ILE:HD13	1:A:530:ILE:HG21	1.80	0.41
1:A:657:PRO:HB3	1:A:702:PRO:HD2	2.02	0.41
1:A:703:ILE:HD12	1:A:814:HIS:O	2.20	0.41
1:A:917:LEU:H	1:A:917:LEU:HG	1.79	0.41
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.95	0.41
1:B:326:MET:HE1	1:B:419:LEU:HD11	2.02	0.41
1:B:672:VAL:HA	1:B:675:GLN:HB2	2.03	0.41
1:B:408:PHE:O	1:B:411:PRO:HD2	2.21	0.41
1:B:777:TRP:HA	1:B:780:THR:HG22	2.02	0.41
1:A:115:TYR:O	1:A:119:ILE:HG22	2.21	0.40
1:A:587:ILE:HD13	1:A:587:ILE:HA	1.74	0.40
1:B:98:PHE:CZ	1:B:896:THR:HG21	2.56	0.40
1:B:174:PRO:HB3	1:B:753:GLY:HA3	2.03	0.40
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.93	0.40
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.40
1:B:201:ILE:O	1:B:201:ILE:HG12	2.20	0.40
1:A:168:LEU:O	1:A:281:PHE:HA	2.21	0.40
1:A:546:GLN:OE1	1:A:555:LEU:N	2.53	0.40
1:A:672:VAL:O	1:A:676:SER:OG	2.38	0.40
1:A:712:LEU:O	1:A:716:MET:HB2	2.21	0.40
1:A:798:ILE:HG12	1:A:798:ILE:H	1.69	0.40
1:B:621:VAL:HG21	1:B:659:THR:HA	2.02	0.40
1:B:801:ASP:OD2	1:B:803:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	899/974 (92%)	849 (94%)	44 (5%)	6 (1%)	18	50
1	B	880/974 (90%)	832 (94%)	43 (5%)	5 (1%)	21	53
All	All	1779/1948 (91%)	1681 (94%)	87 (5%)	11 (1%)	21	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	GLY
1	A	918	ARG
1	A	919	PRO
1	B	670	GLY
1	B	889	LEU
1	A	848	GLU
1	A	911	PRO
1	B	848	GLU
1	B	888	ARG
1	B	911	PRO
1	A	119	ILE

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	779/850 (92%)	722 (93%)	57 (7%)	13	41
1	B	769/850 (90%)	715 (93%)	54 (7%)	14	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1548/1700 (91%)	1437 (93%)	111 (7%)	13	41

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	71	HIS
1	A	79	LEU
1	A	102	LEU
1	A	117	ARG
1	A	165	THR
1	A	169	VAL
1	A	175	THR
1	A	182	LEU
1	A	196	LEU
1	A	201	ILE
1	A	228	ARG
1	A	229	THR
1	A	237	MET
1	A	256	LEU
1	A	269	GLU
1	A	279	ILE
1	A	306	LEU
1	A	308	ARG
1	A	309	MET
1	A	318	GLN
1	A	319	ILE
1	A	332	ASN
1	A	345	ASN
1	A	348	LYS
1	A	359	LYS
1	A	365	GLU
1	A	388	LEU
1	A	393	HIS
1	A	399	GLU
1	A	406	GLU
1	A	469	LEU
1	A	480	GLU
1	A	497	PHE
1	A	504	THR
1	A	510	VAL
1	A	552	LYS

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Mol	Chain	Res	Type
1	A	555	LEU
1	A	558	VAL
1	A	567	LEU
1	A	587	ILE
1	A	632	THR
1	A	688	GLN
1	A	713	LEU
1	A	723	GLU
1	A	727	VAL
1	A	767	SER
1	A	768	LEU
1	A	771	ILE
1	A	798	ILE
1	A	799	GLU
1	A	849	LEU
1	A	887	LEU
1	A	889	LEU
1	A	917	LEU
1	A	930	LYS
1	A	954	LEU
1	B	33	TYR
1	B	71	HIS
1	B	102	LEU
1	B	117	ARG
1	B	165	THR
1	B	169	VAL
1	B	182	LEU
1	B	196	LEU
1	B	201	ILE
1	B	228	ARG
1	B	237	MET
1	B	256	LEU
1	B	269	GLU
1	B	278	LEU
1	B	279	ILE
1	B	285	MET
1	B	306	LEU
1	B	309	MET
1	B	318	GLN
1	B	319	ILE
1	B	320	GLU
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	345	ASN
1	B	348	LYS
1	B	359	LYS
1	B	365	GLU
1	B	378	LEU
1	B	388	LEU
1	B	393	HIS
1	B	399	GLU
1	B	406	GLU
1	B	469	LEU
1	B	493	LYS
1	B	497	PHE
1	B	504	THR
1	B	510	VAL
1	B	552	LYS
1	B	555	LEU
1	B	558	VAL
1	B	567	LEU
1	B	587	ILE
1	B	632	THR
1	B	688	GLN
1	B	713	LEU
1	B	723	GLU
1	B	727	VAL
1	B	767	SER
1	B	771	ILE
1	B	798	ILE
1	B	799	GLU
1	B	849	LEU
1	B	887	LEU
1	B	934	GLU
1	B	954	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	407	GLN
1	A	661	ASN
1	A	914	HIS
1	A	939	ASN
1	B	46	GLN

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Mol	Chain	Res	Type
1	B	100	HIS
1	B	186	HIS
1	B	332	ASN
1	B	661	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](#)

2 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	PO4	B	1001	-	4,4,4	1.03	0	6,6,6	0.48	0
2	PO4	A	1001	-	4,4,4	1.33	0	6,6,6	0.52	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PO4	1	0
2	A	1001	PO4	2	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	906/974 (93%)	-0.21	22 (2%)	59 40	48, 95, 156, 252	3 (0%)
1	B	890/974 (91%)	-0.03	30 (3%)	48 30	91, 168, 241, 297	0
All	All	1796/1948 (92%)	-0.13	52 (2%)	53 35	48, 126, 227, 297	3 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	LEU	5.0
1	B	193	LEU	4.4
1	A	761	PRO	4.3
1	A	636	GLY	4.2
1	B	771	ILE	4.1
1	B	830	ALA	4.0
1	B	815	TRP	3.5
1	A	136	GLU	3.5
1	B	281	PHE	3.4
1	B	279	ILE	3.2
1	B	824	LEU	3.2
1	A	245	HIS	3.1
1	A	405	LEU	3.1
1	B	608	SER	3.1
1	B	692	ALA	3.0
1	A	638	GLY	2.9
1	A	88	PRO	2.8
1	A	178	VAL	2.8
1	A	82	VAL	2.7
1	A	763	GLY	2.7
1	B	650	LEU	2.7
1	B	826	GLU	2.6
1	A	764	GLY	2.6
1	A	785	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	764	GLY	2.5
1	B	190	ARG	2.5
1	B	37	LEU	2.5
1	A	875	ASP	2.5
1	A	78	GLU	2.4
1	B	827	MET	2.4
1	B	954	LEU	2.4
1	A	967	GLY	2.3
1	B	818	PHE	2.3
1	B	221	PHE	2.3
1	B	632	THR	2.3
1	B	107	LEU	2.2
1	A	921	ILE	2.2
1	B	677	PHE	2.2
1	A	709	TRP	2.1
1	A	597	TYR	2.1
1	A	606[A]	ARG	2.1
1	A	601	GLY	2.1
1	B	705	PRO	2.1
1	B	790	PHE	2.1
1	B	687	LEU	2.1
1	A	680	GLU	2.1
1	B	245	HIS	2.1
1	B	601	GLY	2.1
1	A	703	ILE	2.0
1	B	642	GLY	2.0
1	B	88	PRO	2.0
1	B	104	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 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	PO4	B	1001	5/5	0.89	0.13	181,185,189,199	0
2	PO4	A	1001	5/5	0.94	0.08	121,126,131,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.