



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:03 AM UTC

PDB ID : 8S5F / pdb_00008s5f
Title : Crystal structure of the HExxH domain of ChlBHExxH a novel alpha-ketoglutarate dependent oxygenase
Authors : de la Mora, E.; Amara, P.; Usclat, A.; Morishita, Y.; Morinaka, B.; Nicolet, Y.
Deposited on : 2024-02-23
Resolution : 2.80 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

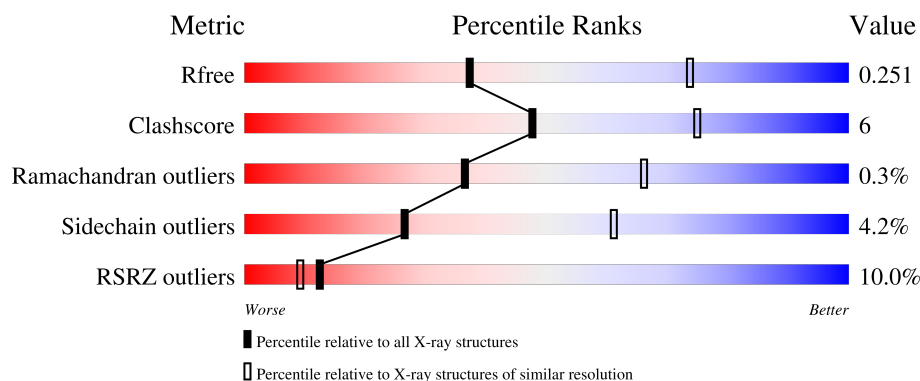
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	368	5% 80% 12% • 7%
1	B	368	8% 77% 14% • 7%
1	C	368	9% 79% 12% • 7%
1	D	368	14% 76% 13% • 9%
1	E	368	8% 76% 13% 10%

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Mol	Chain	Length	Quality of chain
1	F	368	11% 74% 12% • 13%

2 Entry composition [i](#)

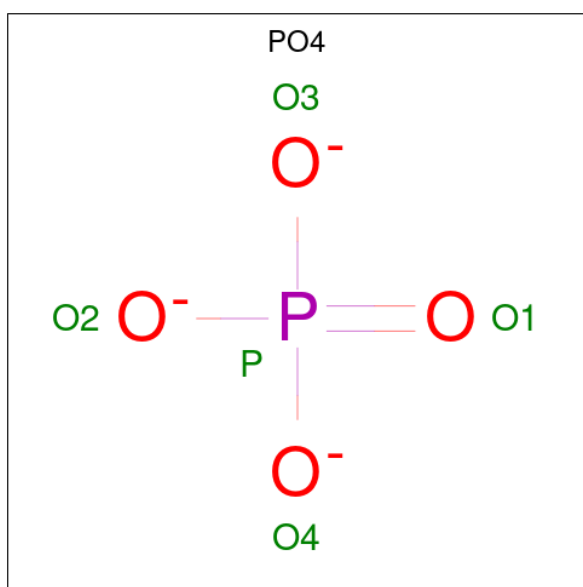
There are 2 unique types of molecules in this entry. The entry contains 16156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ChlH from Chlorogloeopsis sp..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	3	0
			2747	1753	475	513	6			
1	B	342	Total	C	N	O	S	0	1	0
			2741	1749	474	512	6			
1	C	342	Total	C	N	O	S	0	0	0
			2735	1746	473	510	6			
1	D	335	Total	C	N	O	S	0	0	0
			2682	1715	465	496	6			
1	E	331	Total	C	N	O	S	0	0	0
			2650	1700	452	493	5			
1	F	320	Total	C	N	O	S	0	0	0
			2571	1648	440	478	5			

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

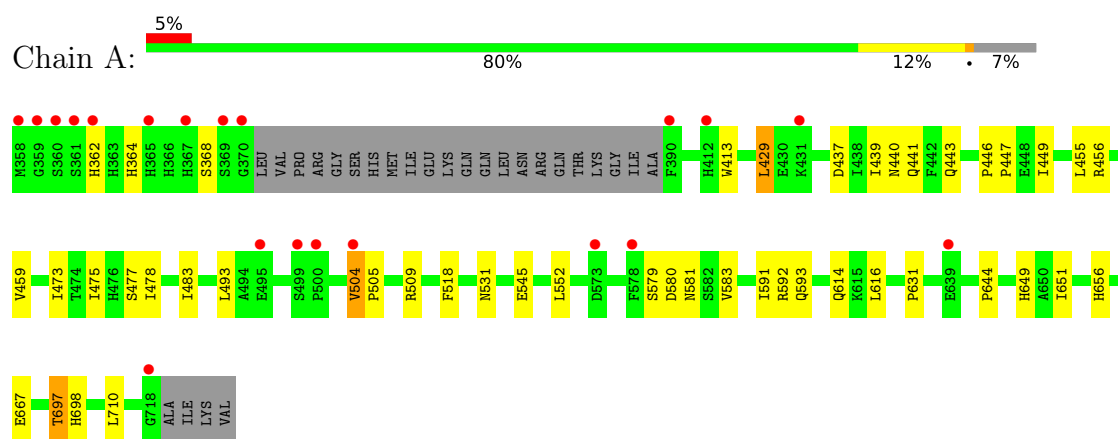


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

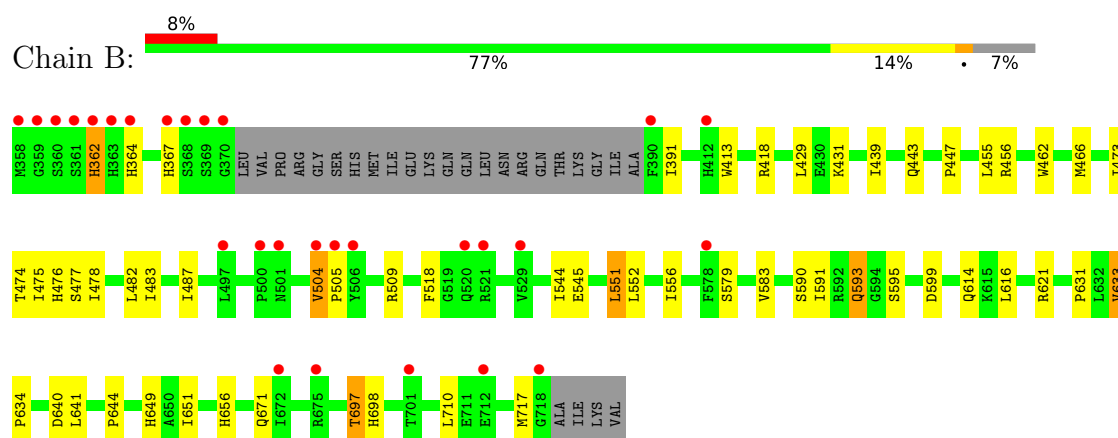
3 Residue-property plots [i](#)

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.

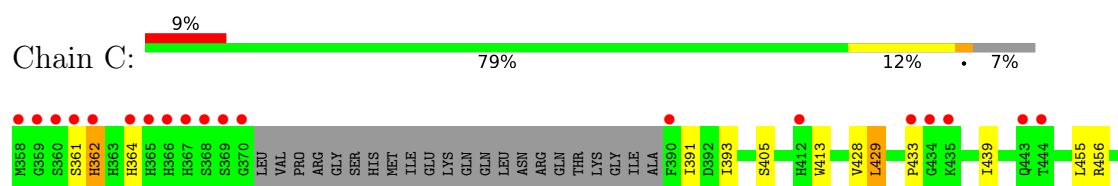
- Molecule 1: ChlH from *Chlorogloeopsis* sp.

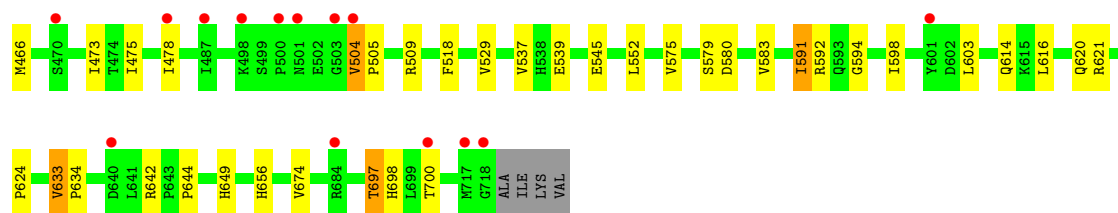


- Molecule 1: ChlH from *Chlorogloeopsis* sp.

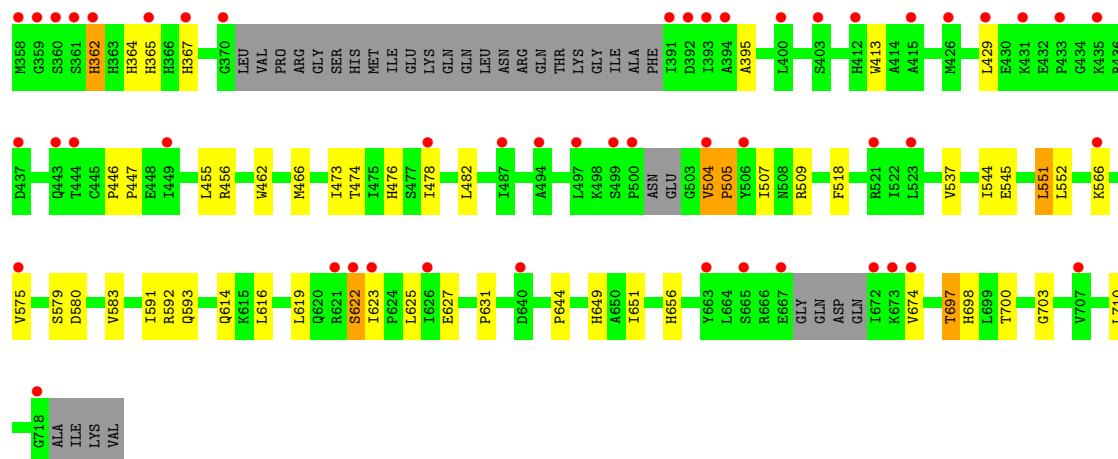
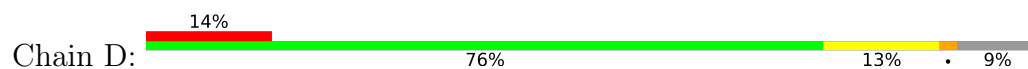


- Molecule 1: ChlH from *Chlorogloeopsis* sp.

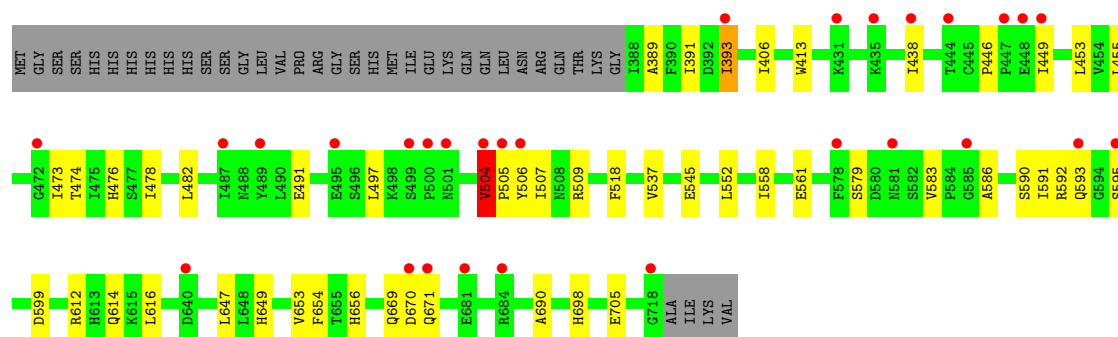
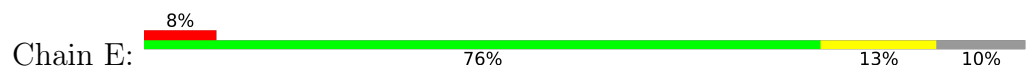




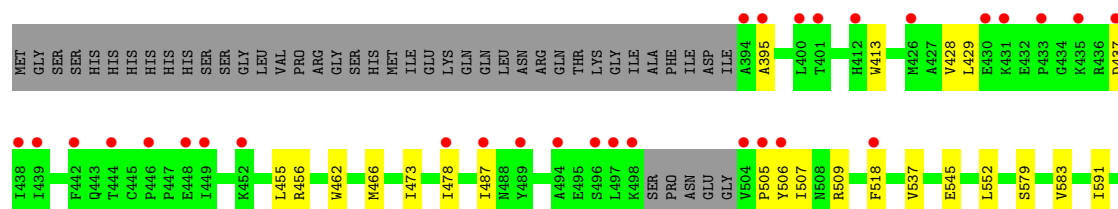
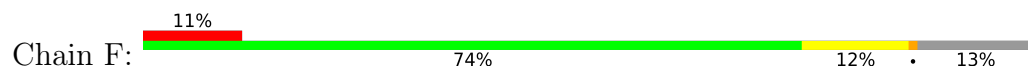
- Molecule 1: ChlH from Chlorogloeopsis sp.

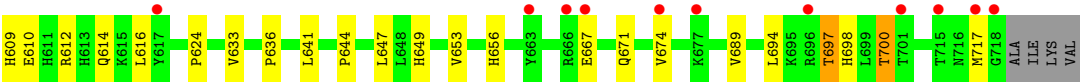


- Molecule 1: ChlH from Chlorogloeopsis sp.



- Molecule 1: ChlH from Chlorogloeopsis sp.





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.42Å 86.99Å 198.23Å 90.00° 95.76° 90.00°	Depositor
Resolution (Å)	69.56 – 2.80 69.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	60.1 (69.56-2.80) 60.0 (69.56-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.235 , 0.255 (Not available) , 0.251	Depositor DCC
R_{free} test set	2928 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	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	0.91	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.61	0/2816	1.01	1/3829 (0.0%)
1	B	0.60	0/2805	1.03	1/3815 (0.0%)
1	C	0.59	0/2799	1.01	1/3807 (0.0%)
1	D	0.59	0/2744	1.03	2/3730 (0.1%)
1	E	0.57	0/2710	0.99	3/3690 (0.1%)
1	F	0.55	0/2628	0.99	2/3576 (0.1%)
All	All	0.58	0/16502	1.01	10/22447 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	395	ALA	CA-C-N	7.16	130.84	120.38
1	F	395	ALA	C-N-CA	7.16	130.84	120.38
1	C	594	GLY	N-CA-C	-5.87	106.27	111.67
1	D	395	ALA	CA-C-N	5.66	128.43	120.28
1	D	395	ALA	C-N-CA	5.66	128.43	120.28
1	B	362	HIS	N-CA-C	5.33	119.41	113.02
1	E	654	PHE	CA-CB-CG	-5.15	108.65	113.80
1	E	389	ALA	N-CA-C	5.08	117.03	109.25
1	E	391	ILE	N-CA-C	5.05	115.76	108.48
1	A	362	HIS	N-CA-C	5.02	119.05	113.02

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	2747	0	2754	31	0
1	B	2741	0	2741	44	0
1	C	2735	0	2737	37	0
1	D	2682	0	2696	43	0
1	E	2650	0	2680	38	0
1	F	2571	0	2603	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
All	All	16156	0	16211	180	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 6.

All (180) 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:504:VAL:HG23	1:B:505:PRO:HD3	1.57	0.86
1:E:473:ILE:HD13	1:F:698:HIS:CE1	2.12	0.84
1:E:474:THR:HG22	1:E:476:HIS:CE1	2.13	0.83
1:B:671:GLN:HE22	1:E:592:ARG:HH12	1.28	0.82
1:D:474:THR:HG22	1:D:476:HIS:CE1	2.14	0.81
1:A:473:ILE:HD13	1:B:698:HIS:CE1	2.19	0.77
1:A:504:VAL:HG23	1:A:505:PRO:HD3	1.65	0.76
1:C:504:VAL:HB	1:C:505:PRO:HD3	1.67	0.75
1:D:474:THR:HG23	1:D:482:LEU:HD13	1.69	0.74
1:E:474:THR:HG23	1:E:482:LEU:HD13	1.69	0.73
1:B:456:ARG:NH2	1:B:509:ARG:HH12	1.87	0.72
1:B:474:THR:HG23	1:B:482:LEU:HD13	1.73	0.71
1:B:671:GLN:HE22	1:E:592:ARG:NH1	1.91	0.69
1:C:504:VAL:HB	1:C:505:PRO:CD	2.23	0.69
1:A:579[B]:SER:OG	1:A:614:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ARG:NH2	1:D:509:ARG:HH12	1.91	0.68
1:B:474:THR:HG22	1:B:476:HIS:NE2	2.08	0.67
1:C:473:ILE:HD13	1:D:698:HIS:CE1	2.29	0.66
1:A:698:HIS:CE1	1:B:473:ILE:HD13	2.30	0.66
1:A:456:ARG:NH2	1:A:509:ARG:HH12	1.93	0.66
1:C:456:ARG:NH2	1:C:509:ARG:HH12	1.94	0.65
1:D:566:LYS:NZ	1:D:592:ARG:HH21	1.95	0.65
1:E:438:ILE:HD13	1:E:491:GLU:HG2	1.78	0.65
1:D:566:LYS:NZ	1:D:592:ARG:NH2	2.45	0.64
1:E:698:HIS:NE2	1:F:473:ILE:HD13	2.12	0.63
1:E:474:THR:CG2	1:E:476:HIS:CE1	2.82	0.62
1:F:456:ARG:NH2	1:F:509:ARG:HH12	1.98	0.62
1:A:440:ASN:HD22	1:A:443:GLN:NE2	1.98	0.61
1:A:413:TRP:CD2	1:A:455:LEU:HD22	2.35	0.61
1:F:413:TRP:CD2	1:F:455:LEU:HD22	2.36	0.61
1:A:473:ILE:HD13	1:B:698:HIS:NE2	2.15	0.61
1:C:413:TRP:CD2	1:C:455:LEU:HD22	2.35	0.61
1:B:579:SER:HB2	1:B:614:GLN:NE2	2.15	0.61
1:D:413:TRP:CD2	1:D:455:LEU:HD22	2.35	0.61
1:D:627:GLU:HG2	1:D:700:THR:HG22	1.83	0.61
1:D:474:THR:CG2	1:D:476:HIS:CE1	2.84	0.61
1:B:413:TRP:CD2	1:B:455:LEU:HD22	2.37	0.60
1:D:579:SER:HB2	1:D:614:GLN:NE2	2.17	0.60
1:E:413:TRP:CD2	1:E:455:LEU:HD22	2.36	0.60
1:E:579:SER:HB2	1:E:614:GLN:NE2	2.16	0.60
1:B:590:SER:OG	1:B:593:GLN:NE2	2.34	0.60
1:F:579:SER:HB2	1:F:614:GLN:NE2	2.16	0.60
1:A:698:HIS:NE2	1:B:473:ILE:HD13	2.18	0.59
1:E:698:HIS:NE2	1:F:473:ILE:CD1	2.65	0.59
1:C:473:ILE:HD13	1:D:698:HIS:NE2	2.18	0.58
1:B:579:SER:HB2	1:B:614:GLN:HE21	1.69	0.58
1:A:456:ARG:NH2	1:A:509:ARG:NH1	2.52	0.58
1:C:579:SER:HB2	1:C:614:GLN:NE2	2.18	0.57
1:C:621:ARG:NH1	1:D:367:HIS:CD2	2.71	0.57
1:C:456:ARG:NH2	1:C:509:ARG:NH1	2.52	0.57
1:E:579:SER:HB2	1:E:614:GLN:HE21	1.68	0.57
1:F:579:SER:HB2	1:F:614:GLN:HE21	1.69	0.57
1:D:456:ARG:NH2	1:D:509:ARG:NH1	2.52	0.57
1:C:698:HIS:NE2	1:D:473:ILE:HD13	2.19	0.56
1:C:429:LEU:HD12	1:C:433:PRO:HA	1.88	0.56
1:C:579:SER:HB2	1:C:614:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:SER:HB3	1:A:483:ILE:HD11	1.87	0.56
1:B:456:ARG:NH2	1:B:509:ARG:NH1	2.52	0.55
1:C:624:PRO:O	1:C:700:THR:HG21	2.06	0.55
1:E:473:ILE:CD1	1:F:698:HIS:NE2	2.69	0.55
1:E:504:VAL:HB	1:E:505:PRO:HD3	1.88	0.55
1:F:624:PRO:O	1:F:700:THR:HG21	2.07	0.55
1:C:580:ASP:HA	1:D:362:HIS:HB2	1.89	0.55
1:D:507:ILE:HD12	1:D:537:VAL:HG11	1.89	0.55
1:F:456:ARG:NH2	1:F:509:ARG:NH1	2.55	0.55
1:D:579:SER:HB2	1:D:614:GLN:HE21	1.70	0.54
1:C:620:GLN:HE21	1:D:367:HIS:HE1	1.54	0.54
1:A:429:LEU:HD12	1:A:439:ILE:HD13	1.89	0.54
1:C:429:LEU:HD13	1:C:439:ILE:HD12	1.90	0.54
1:E:590:SER:OG	1:E:593:GLN:NE2	2.40	0.54
1:D:619:LEU:O	1:D:622:SER:O	2.26	0.53
1:D:566:LYS:HZ3	1:D:592:ARG:NH2	2.06	0.52
1:E:473:ILE:HD13	1:F:698:HIS:NE2	2.24	0.52
1:B:504:VAL:HB	1:B:556:ILE:HG23	1.91	0.52
1:D:478:ILE:HG12	1:D:518:PHE:HA	1.92	0.52
1:C:698:HIS:CD2	1:D:473:ILE:HD13	2.45	0.51
1:A:473:ILE:CD1	1:B:698:HIS:NE2	2.73	0.51
1:E:478:ILE:HG12	1:E:518:PHE:HA	1.91	0.51
1:C:698:HIS:CE1	1:D:473:ILE:CD1	2.94	0.51
1:E:616:LEU:HD23	1:E:649:HIS:CD2	2.45	0.51
1:D:413:TRP:CE2	1:D:455:LEU:HD22	2.46	0.51
1:F:478:ILE:HG12	1:F:518:PHE:HA	1.93	0.51
1:F:636:PRO:HG3	1:F:689:VAL:HG23	1.93	0.51
1:A:413:TRP:CE2	1:A:455:LEU:HD22	2.45	0.51
1:C:478:ILE:HG12	1:C:518:PHE:HA	1.92	0.51
1:B:478:ILE:HG12	1:B:518:PHE:HA	1.92	0.50
1:D:566:LYS:HZ3	1:D:592:ARG:HH21	1.59	0.50
1:E:474:THR:HG23	1:E:482:LEU:CD1	2.40	0.50
1:A:478:ILE:HG12	1:A:518:PHE:HA	1.92	0.50
1:B:595:SER:O	1:E:599:ASP:OD2	2.29	0.50
1:D:566:LYS:HZ2	1:D:592:ARG:NH2	2.09	0.50
1:E:413:TRP:CE2	1:E:455:LEU:HD22	2.46	0.50
1:F:413:TRP:CE2	1:F:455:LEU:HD22	2.45	0.50
1:F:462:TRP:CE2	1:F:466:MET:HE3	2.46	0.50
1:C:413:TRP:CE2	1:C:455:LEU:HD22	2.46	0.50
1:E:507:ILE:HD12	1:E:537:VAL:HG11	1.93	0.50
1:F:616:LEU:HD23	1:F:649:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:TRP:CE2	1:B:455:LEU:HD22	2.47	0.50
1:B:671:GLN:NE2	1:E:592:ARG:NH1	2.59	0.50
1:D:462:TRP:CE2	1:D:466:MET:HE3	2.47	0.50
1:B:462:TRP:CE2	1:B:466:MET:HE3	2.47	0.49
1:A:579[A]:SER:HB2	1:A:614:GLN:NE2	2.28	0.49
1:B:474:THR:CG2	1:B:476:HIS:NE2	2.74	0.49
1:D:625:LEU:HD23	1:D:703:GLY:HA2	1.96	0.48
1:B:418:ARG:NH2	1:B:447:PRO:HB3	2.29	0.48
1:E:698:HIS:CD2	1:F:473:ILE:HD13	2.49	0.48
1:A:616:LEU:HD23	1:A:649:HIS:CD2	2.49	0.48
1:C:616:LEU:HD23	1:C:649:HIS:CD2	2.49	0.48
1:B:616:LEU:HD23	1:B:649:HIS:CD2	2.49	0.48
1:A:580:ASP:HA	1:B:362:HIS:HB3	1.95	0.48
1:F:428:VAL:HG22	1:F:487:ILE:HG22	1.96	0.48
1:B:633:VAL:HG22	1:B:634:PRO:HD2	1.96	0.48
1:C:598:ILE:HD11	1:C:603:LEU:HD13	1.96	0.47
1:D:474:THR:HG23	1:D:482:LEU:CD1	2.41	0.47
1:D:616:LEU:HD23	1:D:649:HIS:CD2	2.49	0.47
1:E:506:TYR:CD2	1:E:509:ARG:NH1	2.80	0.47
1:E:698:HIS:CE1	1:F:473:ILE:HD11	2.50	0.47
1:D:544:ILE:HG23	1:D:551:LEU:HD12	1.95	0.47
1:B:544:ILE:HG23	1:B:551:LEU:HD12	1.97	0.47
1:A:459:VAL:HG22	1:A:493:LEU:HD11	1.96	0.46
1:C:473:ILE:CD1	1:D:698:HIS:NE2	2.79	0.46
1:B:474:THR:HG23	1:B:482:LEU:CD1	2.43	0.46
1:C:621:ARG:HH11	1:D:367:HIS:CD2	2.32	0.46
1:B:644:PRO:HB3	1:B:697:THR:HG21	1.98	0.46
1:C:620:GLN:HE21	1:D:367:HIS:CE1	2.35	0.45
1:C:644:PRO:HB3	1:C:697:THR:HG21	1.98	0.45
1:F:644:PRO:HB3	1:F:697:THR:HG21	1.99	0.45
1:B:474:THR:CG2	1:B:476:HIS:CE1	2.99	0.45
1:E:545:GLU:HB2	1:E:552:LEU:HD22	1.99	0.45
1:E:698:HIS:CE1	1:F:473:ILE:CD1	2.99	0.45
1:C:473:ILE:CD1	1:D:698:HIS:CD2	2.99	0.45
1:E:647:LEU:HD11	1:E:690:ALA:HB1	1.99	0.45
1:C:475:ILE:HG12	1:D:631:PRO:HG3	1.99	0.44
1:D:504:VAL:HG13	1:D:505:PRO:HD2	2.00	0.44
1:F:612:ARG:HB2	1:F:653:VAL:HG22	1.99	0.44
1:A:698:HIS:NE2	1:B:473:ILE:CD1	2.79	0.44
1:C:545:GLU:HB2	1:C:552:LEU:HD22	1.99	0.44
1:D:644:PRO:HB3	1:D:697:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ILE:CD1	1:B:698:HIS:CD2	3.00	0.43
1:C:391:ILE:HD11	1:C:405:SER:HB3	2.00	0.43
1:A:644:PRO:HB3	1:A:697:THR:HG21	1.99	0.43
1:A:651:ILE:HG22	1:A:710:LEU:HD13	2.00	0.43
1:C:529:VAL:CG1	1:C:592:ARG:HD2	2.49	0.43
1:E:504:VAL:CB	1:E:505:PRO:HD3	2.47	0.43
1:A:440:ASN:ND2	1:A:443:GLN:NE2	2.66	0.43
1:F:545:GLU:HB2	1:F:552:LEU:HD22	1.99	0.43
1:B:474:THR:HG21	1:B:476:HIS:CE1	2.54	0.43
1:A:545:GLU:HB2	1:A:552:LEU:HD22	2.00	0.43
1:A:581:ASN:ND2	1:B:367:HIS:ND1	2.66	0.43
1:D:545:GLU:HB2	1:D:552:LEU:HD22	2.00	0.43
1:F:505:PRO:O	1:F:507:ILE:HG13	2.19	0.43
1:E:393:ILE:HD11	1:E:705:GLU:HB3	2.01	0.42
1:B:477:SER:HB3	1:B:483:ILE:HD11	2.01	0.42
1:E:453:LEU:HD22	1:E:497:LEU:HD21	2.00	0.42
1:E:473:ILE:CD1	1:F:698:HIS:CE1	2.94	0.42
1:D:504:VAL:O	1:D:505:PRO:C	2.62	0.42
1:B:651:ILE:HG22	1:B:710:LEU:HD13	2.02	0.42
1:C:362:HIS:HB2	1:D:580:ASP:HA	2.01	0.42
1:B:431:LYS:HE3	1:B:487:ILE:HD11	2.00	0.42
1:E:446:PRO:HD2	1:E:449:ILE:HD12	2.02	0.42
1:B:545:GLU:HB2	1:B:552:LEU:HD22	2.00	0.41
1:D:651:ILE:HG22	1:D:710:LEU:HD13	2.02	0.41
1:D:446:PRO:HA	1:D:447:PRO:HD3	1.98	0.41
1:A:446:PRO:HA	1:A:447:PRO:HD3	1.98	0.41
1:C:633:VAL:HG22	1:C:634:PRO:HD2	2.01	0.41
1:E:406:ILE:HD13	1:E:558:ILE:HD11	2.03	0.41
1:A:531:ASN:ND2	1:C:539:GLU:OE2	2.54	0.41
1:E:561:GLU:HB2	1:E:586:ALA:HA	2.02	0.41
1:A:475:ILE:HG12	1:B:631:PRO:HG3	2.01	0.41
1:C:642:ARG:HD2	1:C:642:ARG:HA	1.96	0.41
1:B:599:ASP:OD2	1:E:595:SER:O	2.39	0.41
1:C:428:VAL:HG23	1:C:466:MET:HE2	2.03	0.41
1:C:529:VAL:HG12	1:C:591:ILE:HD11	2.03	0.41
1:F:647:LEU:HD23	1:F:694:LEU:HB2	2.02	0.41
1:B:439:ILE:O	1:B:443:GLN:HG3	2.21	0.41
1:A:446:PRO:HD2	1:A:449:ILE:HD12	2.02	0.40
1:A:631:PRO:HG3	1:B:475:ILE:HG12	2.02	0.40
1:B:456:ARG:HH21	1:B:509:ARG:HH12	1.61	0.40
1:F:609:HIS:CD2	1:F:610:GLU:OE2	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:612:ARG:HB2	1:E:653:VAL:HG22	2.04	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	341/368 (93%)	326 (96%)	15 (4%)	0	100	100
1	B	339/368 (92%)	321 (95%)	18 (5%)	0	100	100
1	C	338/368 (92%)	320 (95%)	17 (5%)	1 (0%)	36	66
1	D	327/368 (89%)	308 (94%)	16 (5%)	3 (1%)	14	41
1	E	329/368 (89%)	320 (97%)	8 (2%)	1 (0%)	36	66
1	F	316/368 (86%)	308 (98%)	7 (2%)	1 (0%)	36	66
All	All	1990/2208 (90%)	1903 (96%)	81 (4%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	504	VAL
1	E	504	VAL
1	F	506	TYR
1	D	505	PRO
1	D	504	VAL
1	D	623	ILE

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	307/328 (94%)	294 (96%)	13 (4%)	26	61
1	B	306/328 (93%)	291 (95%)	15 (5%)	22	55
1	C	305/328 (93%)	292 (96%)	13 (4%)	26	60
1	D	300/328 (92%)	287 (96%)	13 (4%)	26	60
1	E	295/328 (90%)	287 (97%)	8 (3%)	39	74
1	F	287/328 (88%)	273 (95%)	14 (5%)	22	55
All	All	1800/1968 (92%)	1724 (96%)	76 (4%)	26	61

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	A	368	SER
1	A	429	LEU
1	A	437	ASP
1	A	441	GLN
1	A	504	VAL
1	A	583	VAL
1	A	591	ILE
1	A	592	ARG
1	A	593	GLN
1	A	656	HIS
1	A	667	GLU
1	A	697	THR
1	B	364	HIS
1	B	391	ILE
1	B	429	LEU
1	B	504	VAL
1	B	551	LEU
1	B	583	VAL
1	B	591	ILE
1	B	593	GLN
1	B	621	ARG
1	B	633	VAL
1	B	640	ASP
1	B	641	LEU
1	B	656	HIS

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Mol	Chain	Res	Type
1	B	697	THR
1	B	717	MET
1	C	361	SER
1	C	362	HIS
1	C	364	HIS
1	C	393	ILE
1	C	429	LEU
1	C	537	VAL
1	C	575	VAL
1	C	583	VAL
1	C	591	ILE
1	C	633	VAL
1	C	656	HIS
1	C	674	VAL
1	C	697	THR
1	D	362	HIS
1	D	364	HIS
1	D	365	HIS
1	D	429	LEU
1	D	551	LEU
1	D	575	VAL
1	D	583	VAL
1	D	591	ILE
1	D	593	GLN
1	D	622	SER
1	D	656	HIS
1	D	674	VAL
1	D	697	THR
1	E	393	ILE
1	E	504	VAL
1	E	583	VAL
1	E	591	ILE
1	E	656	HIS
1	E	669	GLN
1	E	670	ASP
1	E	671	GLN
1	F	429	LEU
1	F	437	ASP
1	F	537	VAL
1	F	583	VAL
1	F	591	ILE
1	F	633	VAL

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Mol	Chain	Res	Type
1	F	641	LEU
1	F	656	HIS
1	F	667	GLU
1	F	671	GLN
1	F	674	VAL
1	F	697	THR
1	F	700	THR
1	F	717	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	A	468	GLN
1	A	581	ASN
1	A	609	HIS
1	B	468	GLN
1	B	488	ASN
1	B	563	GLN
1	B	581	ASN
1	B	609	HIS
1	B	671	GLN
1	B	698	HIS
1	C	476	HIS
1	C	488	ASN
1	C	571	HIS
1	C	581	ASN
1	C	593	GLN
1	C	620	GLN
1	D	581	ASN
1	D	609	HIS
1	D	620	GLN
1	E	407	GLN
1	E	440	ASN
1	E	571	HIS
1	E	609	HIS
1	F	407	GLN
1	F	440	ASN
1	F	593	GLN
1	F	671	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	C	801	-	4,4,4	0.24	0	6,6,6	0.31	0
2	PO4	A	801	-	4,4,4	0.28	0	6,6,6	0.32	0
2	PO4	B	801	-	4,4,4	0.19	0	6,6,6	0.37	0
2	PO4	F	801	-	4,4,4	0.14	0	6,6,6	0.33	0
2	PO4	E	801	-	4,4,4	0.20	0	6,6,6	0.31	0
2	PO4	D	801	-	4,4,4	0.25	0	6,6,6	0.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	342/368 (92%)	0.42	20 (5%)	29 22	23, 57, 83, 98	8 (2%)
1	B	342/368 (92%)	0.59	28 (8%)	17 13	39, 63, 93, 100	5 (1%)
1	C	342/368 (92%)	0.68	33 (9%)	13 10	49, 71, 105, 116	3 (0%)
1	D	335/368 (91%)	1.20	50 (14%)	5 4	66, 86, 116, 131	3 (0%)
1	E	331/368 (89%)	0.81	29 (8%)	15 11	50, 73, 118, 125	0
1	F	320/368 (86%)	1.13	41 (12%)	7 6	73, 96, 134, 144	0
All	All	2012/2208 (91%)	0.80	201 (9%)	12 9	23, 74, 116, 144	19 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	391	ILE	7.8
1	D	500	PRO	7.1
1	D	361	SER	6.4
1	A	361	SER	6.2
1	F	394	ALA	6.1
1	F	487	ILE	6.0
1	A	370	GLY	6.0
1	B	361	SER	5.5
1	D	370	GLY	5.3
1	C	370	GLY	5.2
1	C	361	SER	5.1
1	E	504	VAL	5.1
1	B	390	PHE	4.8
1	A	359	GLY	4.7
1	A	362	HIS	4.6
1	F	400	LEU	4.6
1	C	365	HIS	4.4
1	B	362	HIS	4.4
1	C	358	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	501	ASN	4.3
1	A	504	VAL	4.2
1	D	393	ILE	4.1
1	A	367	HIS	4.1
1	D	494	ALA	4.1
1	C	368	SER	4.1
1	A	500	PRO	4.1
1	D	504	VAL	4.0
1	D	358	MET	4.0
1	E	438	ILE	3.9
1	D	497	LEU	3.9
1	D	359	GLY	3.9
1	C	504	VAL	3.9
1	B	367	HIS	3.9
1	C	367	HIS	3.8
1	D	362	HIS	3.8
1	B	718	GLY	3.8
1	C	640	ASP	3.7
1	F	663	TYR	3.7
1	F	504	VAL	3.7
1	B	500	PRO	3.6
1	B	504	VAL	3.6
1	D	394	ALA	3.6
1	D	367	HIS	3.5
1	E	472	GLY	3.5
1	D	426	MET	3.5
1	D	718	GLY	3.5
1	D	365	HIS	3.5
1	B	497	LEU	3.5
1	D	400	LEU	3.5
1	C	359	GLY	3.4
1	F	717	MET	3.4
1	C	369	SER	3.4
1	F	505	PRO	3.4
1	B	358	MET	3.4
1	A	360	SER	3.3
1	A	718	GLY	3.3
1	F	478	ILE	3.3
1	A	365	HIS	3.3
1	C	390	PHE	3.3
1	E	500	PRO	3.3
1	B	359	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	500	PRO	3.2
1	F	496	SER	3.2
1	A	390	PHE	3.2
1	D	674	VAL	3.2
1	C	366	HIS	3.1
1	B	501	ASN	3.1
1	A	639	GLU	3.1
1	D	429	LEU	3.0
1	F	431	LYS	3.0
1	E	444	THR	3.0
1	F	401	THR	3.0
1	F	666	ARG	3.0
1	E	578	PHE	3.0
1	A	495	GLU	2.9
1	D	672	ILE	2.9
1	F	433	PRO	2.9
1	E	640	ASP	2.9
1	F	667	GLU	2.8
1	C	435	LYS	2.8
1	C	444	THR	2.8
1	B	578	PHE	2.8
1	B	370	GLY	2.8
1	F	497	LEU	2.8
1	D	431	LYS	2.8
1	F	438	ILE	2.8
1	B	521	ARG	2.8
1	D	521	ARG	2.8
1	C	718	GLY	2.8
1	E	505	PRO	2.7
1	E	393	ILE	2.7
1	F	412	HIS	2.7
1	F	426	MET	2.7
1	C	434	GLY	2.7
1	D	392	ASP	2.7
1	C	443	GLN	2.7
1	A	578	PHE	2.7
1	D	623	ILE	2.6
1	C	360	SER	2.6
1	D	433	PRO	2.6
1	E	487	ILE	2.6
1	D	667	GLU	2.6
1	F	677	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	718	GLY	2.6
1	D	360	SER	2.6
1	E	499	SER	2.6
1	F	494	ALA	2.6
1	A	358	MET	2.6
1	D	506	TYR	2.6
1	D	575	VAL	2.6
1	D	403	SER	2.6
1	E	435	LYS	2.6
1	C	684	ARG	2.5
1	F	452	LYS	2.5
1	C	433	PRO	2.5
1	E	593	GLN	2.5
1	C	412	HIS	2.5
1	F	448	GLU	2.5
1	C	601	TYR	2.5
1	B	360	SER	2.5
1	D	621	ARG	2.5
1	B	364	HIS	2.5
1	C	362	HIS	2.5
1	E	718	GLY	2.5
1	D	707	VAL	2.5
1	C	700	THR	2.4
1	D	523	LEU	2.4
1	C	470	SER	2.4
1	E	595	SER	2.4
1	E	671	GLN	2.4
1	F	395	ALA	2.4
1	E	684	ARG	2.4
1	F	439	ILE	2.4
1	B	712	GLU	2.4
1	B	505	PRO	2.4
1	C	503	GLY	2.4
1	E	431	LYS	2.4
1	B	412	HIS	2.4
1	A	573	ASP	2.4
1	E	448	GLU	2.4
1	E	670	ASP	2.4
1	B	672	ILE	2.4
1	D	626	ILE	2.4
1	E	681	GLU	2.4
1	C	498	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	506	TYR	2.3
1	E	449	ILE	2.3
1	F	449	ILE	2.3
1	D	499	SER	2.3
1	B	506	TYR	2.3
1	C	364	HIS	2.3
1	D	487	ILE	2.3
1	B	701	THR	2.3
1	A	499	SER	2.3
1	B	369[A]	SER	2.3
1	A	412	HIS	2.3
1	D	435	LYS	2.3
1	F	437	ASP	2.3
1	F	435	LYS	2.2
1	D	444	THR	2.2
1	F	715	THR	2.2
1	D	478	ILE	2.2
1	F	498	LYS	2.2
1	F	518	PHE	2.2
1	F	430	GLU	2.2
1	E	581	ASN	2.2
1	E	495	GLU	2.2
1	D	663	TYR	2.2
1	D	566	LYS	2.2
1	F	442	PHE	2.2
1	D	415	ALA	2.2
1	C	501	ASN	2.2
1	F	489	TYR	2.2
1	D	673	LYS	2.2
1	F	674	VAL	2.2
1	B	520	GLN	2.1
1	E	585	GLY	2.1
1	B	363	HIS	2.1
1	C	487	ILE	2.1
1	F	444	THR	2.1
1	E	447	PRO	2.1
1	F	446	PRO	2.1
1	F	617	TYR	2.1
1	D	449	ILE	2.1
1	A	369	SER	2.1
1	A	431	LYS	2.1
1	B	529	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	478	ILE	2.1
1	D	437	ASP	2.1
1	D	640	ASP	2.1
1	D	622	SER	2.1
1	F	696	ARG	2.1
1	F	701	THR	2.1
1	E	489	TYR	2.1
1	B	368	SER	2.0
1	D	443	GLN	2.0
1	D	412	HIS	2.0
1	F	506	TYR	2.0
1	D	665	SER	2.0
1	C	717	MET	2.0
1	B	675	ARG	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(Å ²)	Q<0.9
2	PO4	F	801	5/5	0.68	0.11	128,128,129,129	0
2	PO4	D	801	5/5	0.81	0.13	110,110,110,110	0
2	PO4	E	801	5/5	0.83	0.12	109,109,109,109	0
2	PO4	B	801	5/5	0.85	0.10	78,78,78,78	0
2	PO4	C	801	5/5	0.89	0.08	84,84,84,84	0
2	PO4	A	801	5/5	0.90	0.08	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.