



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:24 PM GMT

PDB ID : 3D8F  
Title : Crystal structure of the human Fe65-PTB1 domain with bound phosphate (trigonal crystal form)  
Authors : Radzimanowski, J.; Ravaud, S.; Sinning, I.; Wild, K.  
Deposited on : 2008-05-23  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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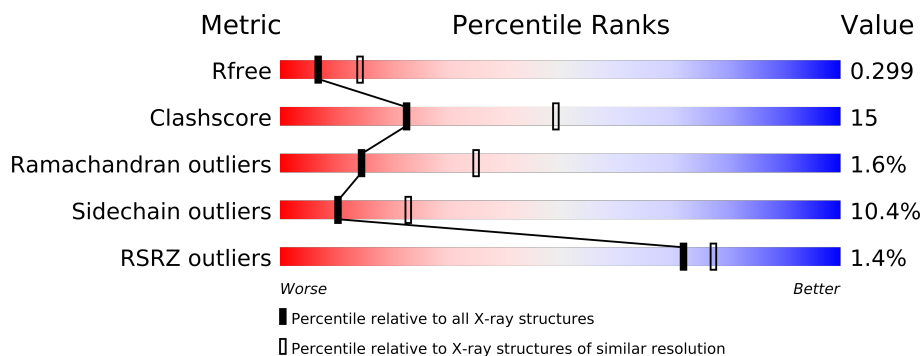
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	148	
1	B	148	
1	C	148	
1	D	148	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4000 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Amyloid beta A4 precursor protein-binding family B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1003	630	180	185	8			
1	B	126	Total	C	N	O	S	0	0	0
			986	622	174	182	8			
1	C	127	Total	C	N	O	S	0	0	0
			1003	630	180	185	8			
1	D	125	Total	C	N	O	S	0	0	0
			976	616	171	181	8			

There are 32 discrepancies between the modelled and reference sequences:

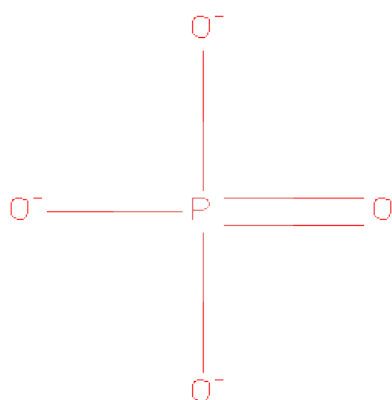
Chain	Residue	Modelled	Actual	Comment	Reference
A	506	LEU	-	EXPRESSION TAG	UNP O00213
A	507	GLU	-	EXPRESSION TAG	UNP O00213
A	508	HIS	-	EXPRESSION TAG	UNP O00213
A	509	HIS	-	EXPRESSION TAG	UNP O00213
A	510	HIS	-	EXPRESSION TAG	UNP O00213
A	511	HIS	-	EXPRESSION TAG	UNP O00213
A	512	HIS	-	EXPRESSION TAG	UNP O00213
A	513	HIS	-	EXPRESSION TAG	UNP O00213
B	506	LEU	-	EXPRESSION TAG	UNP O00213
B	507	GLU	-	EXPRESSION TAG	UNP O00213
B	508	HIS	-	EXPRESSION TAG	UNP O00213
B	509	HIS	-	EXPRESSION TAG	UNP O00213
B	510	HIS	-	EXPRESSION TAG	UNP O00213
B	511	HIS	-	EXPRESSION TAG	UNP O00213
B	512	HIS	-	EXPRESSION TAG	UNP O00213
B	513	HIS	-	EXPRESSION TAG	UNP O00213
C	506	LEU	-	EXPRESSION TAG	UNP O00213
C	507	GLU	-	EXPRESSION TAG	UNP O00213
C	508	HIS	-	EXPRESSION TAG	UNP O00213
C	509	HIS	-	EXPRESSION TAG	UNP O00213

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Chain	Residue	Modelled	Actual	Comment	Reference
C	510	HIS	-	EXPRESSION TAG	UNP O00213
C	511	HIS	-	EXPRESSION TAG	UNP O00213
C	512	HIS	-	EXPRESSION TAG	UNP O00213
C	513	HIS	-	EXPRESSION TAG	UNP O00213
D	506	LEU	-	EXPRESSION TAG	UNP O00213
D	507	GLU	-	EXPRESSION TAG	UNP O00213
D	508	HIS	-	EXPRESSION TAG	UNP O00213
D	509	HIS	-	EXPRESSION TAG	UNP O00213
D	510	HIS	-	EXPRESSION TAG	UNP O00213
D	511	HIS	-	EXPRESSION TAG	UNP O00213
D	512	HIS	-	EXPRESSION TAG	UNP O00213
D	513	HIS	-	EXPRESSION TAG	UNP O00213

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total 5	O 5	0	0
3	C	9	Total 9	O 9	0	0
3	D	4	Total 4	O 4	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.04Å 146.04Å 78.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.21 – 2.70 49.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.21-2.70) 100.0 (49.19-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.242 , 0.313 0.234 , 0.299	Depositor DCC
$R_{free}$ test set	865 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.1	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 17104 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6653e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.71	1/1018 (0.1%)	0.78	0/1371
1	B	0.66	0/1001	0.78	0/1348
1	C	0.72	0/1018	0.77	1/1371 (0.1%)
1	D	0.69	0/990	0.77	0/1333
All	All	0.69	1/4027 (0.0%)	0.78	1/5423 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	CYS	CB-SG	-5.09	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	LEU	CA-CB-CG	5.71	128.43	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1003	0	1017	31	0
1	B	986	0	994	29	0
1	C	1003	0	1017	30	0
1	D	976	0	987	32	0
2	A	5	0	0	0	0
2	C	5	0	0	1	0
3	A	4	0	0	0	0
3	B	5	0	0	1	0
3	C	9	0	0	1	0
3	D	4	0	0	1	0
All	All	4000	0	4015	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:487:PRO:HG2	1:D:490:ASN:ND2	1.95	0.81
1:B:500:SER:O	1:B:503:MET:HB3	1.80	0.81
1:D:502:ILE:O	1:D:505:GLU:HG3	1.81	0.80
1:A:501:LYS:O	1:A:505:GLU:HB2	1.81	0.80
1:B:398:ILE:O	1:B:402:SER:HB2	1.82	0.80
1:D:395:ASN:HB2	3:D:21:HOH:O	1.84	0.77
1:C:385:LEU:HD12	1:C:477:LEU:HD13	1.70	0.72
1:C:436:PRO:O	1:C:439:GLN:NE2	2.23	0.71
1:A:379:GLU:OE1	1:B:367:ILE:HD13	1.91	0.71
1:D:455:VAL:HG23	1:D:456:GLY:N	2.05	0.70
1:D:437:GLN:OE1	1:D:438:SER:HB3	1.93	0.68
1:D:427:GLU:HG3	1:D:432:LYS:HE3	1.76	0.68
1:D:367:ILE:HD12	1:D:427:GLU:HB3	1.75	0.67
1:C:439:GLN:HB2	3:C:16:HOH:O	1.95	0.66
1:C:435:GLU:OE2	1:C:436:PRO:HD2	1.95	0.66
1:C:438:SER:O	1:C:439:GLN:HB2	1.97	0.65
1:C:382:GLU:OE2	1:C:451:ARG:NH2	2.30	0.64
1:A:483:ARG:HG3	1:A:483:ARG:HH11	1.63	0.63
1:B:435:GLU:HG2	1:B:437:GLN:OE1	1.98	0.63
1:B:416:TRP:HB3	1:B:442:LEU:HD12	1.81	0.62
1:A:375:LEU:HD11	1:A:483:ARG:HB2	1.83	0.61
1:D:455:VAL:HG23	1:D:456:GLY:H	1.64	0.60
1:A:429:GLU:C	1:A:447:ILE:HD12	2.22	0.60
1:D:487:PRO:HG2	1:D:490:ASN:HD21	1.65	0.59
1:C:461:ARG:HG2	1:C:461:ARG:HH11	1.67	0.58
1:B:428:ASP:C	1:B:429:GLU:OE1	2.42	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:393:ALA:O	1:B:396:ASN:HB2	2.03	0.57
1:D:367:ILE:HD12	1:D:427:GLU:CB	2.34	0.57
1:C:451:ARG:O	1:C:452:VAL:HG23	2.05	0.57
1:D:476:MET:HG3	1:D:476:MET:O	2.05	0.57
1:B:440:ALA:HA	3:B:12:HOH:O	2.06	0.56
1:D:435:GLU:HG2	1:D:437:GLN:NE2	2.21	0.56
1:C:383:GLU:HB2	1:C:389:ARG:HH22	1.72	0.55
1:A:366:GLY:O	1:A:368:LYS:HG3	2.06	0.55
1:C:470:ARG:NH1	1:C:475:GLN:O	2.39	0.54
1:A:486:ALA:HB1	1:A:487:PRO:HD2	1.90	0.54
1:B:437:GLN:CD	1:B:437:GLN:H	2.11	0.54
1:D:463:ARG:HD2	1:D:484:CYS:O	2.07	0.54
1:B:455:VAL:HG11	1:B:489:LYS:HA	1.90	0.54
1:A:377:TRP:CE3	1:A:478:LYS:HG2	2.42	0.53
1:B:367:ILE:CD1	1:B:367:ILE:N	2.71	0.53
1:D:463:ARG:O	1:D:463:ARG:HG3	2.08	0.53
1:A:502:ILE:O	1:A:506:LEU:HG	2.09	0.53
1:A:436:PRO:O	1:A:439:GLN:NE2	2.41	0.53
1:B:377:TRP:CE2	1:B:478:LYS:HE2	2.45	0.52
1:D:448:ILE:HD13	1:D:502:ILE:HD13	1.92	0.52
1:B:367:ILE:HD12	1:B:367:ILE:N	2.24	0.52
1:A:429:GLU:HA	1:A:447:ILE:HD12	1.92	0.52
1:B:375:LEU:O	1:B:418:GLU:HG3	2.10	0.52
1:A:483:ARG:HG3	1:A:483:ARG:NH1	2.24	0.51
1:D:500:SER:O	1:D:503:MET:HB3	2.10	0.51
1:C:385:LEU:CD1	1:C:477:LEU:HD13	2.39	0.51
1:B:373:ARG:HH11	1:B:373:ARG:HB2	1.75	0.51
1:A:435:GLU:HB3	1:A:438:SER:OG	2.11	0.51
1:C:486:ALA:HB1	1:C:487:PRO:HD2	1.92	0.50
1:B:500:SER:O	1:B:503:MET:CB	2.56	0.50
1:C:461:ARG:HG2	1:C:461:ARG:NH1	2.27	0.50
1:C:461:ARG:N	1:C:462:GLU:OE1	2.45	0.49
1:D:435:GLU:HB2	1:D:442:LEU:HD23	1.94	0.49
1:C:462:GLU:N	1:C:462:GLU:OE1	2.34	0.48
1:D:374:SER:HB3	1:D:417:GLY:O	2.13	0.48
1:D:471:ASP:HB2	1:D:478:LYS:HD2	1.95	0.48
1:C:382:GLU:CD	1:C:451:ARG:HH22	2.17	0.48
1:A:425:GLN:HB2	1:A:432:LYS:HB2	1.96	0.47
1:C:402:SER:HB2	1:C:483:ARG:NH2	2.29	0.47
1:A:369:CYS:SG	1:A:423:LEU:HD22	2.55	0.47
1:C:420:LYS:HG2	1:C:421:ASP:H	1.79	0.47
1:A:403:TYR:HD1	1:B:487:PRO:HG3	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:ARG:HH11	1:A:389:ARG:HG3	1.80	0.46
1:B:367:ILE:H	1:B:367:ILE:CD1	2.29	0.46
1:C:378:VAL:HG23	1:C:401:LEU:HD11	1.97	0.46
1:B:379:GLU:OE2	1:B:476:MET:SD	2.74	0.46
1:D:376:GLY:HA3	1:D:418:GLU:HG2	1.98	0.45
1:B:397:CYS:HA	1:B:400:GLN:HG2	1.97	0.45
1:A:383:GLU:CD	1:A:383:GLU:H	2.20	0.45
1:A:456:GLY:HA3	1:A:461:ARG:HB3	1.99	0.45
1:B:377:TRP:CZ2	1:B:478:LYS:HE2	2.52	0.45
1:D:471:ASP:HB2	1:D:478:LYS:CD	2.47	0.45
1:C:438:SER:O	1:C:439:GLN:CB	2.65	0.45
1:A:429:GLU:CA	1:A:447:ILE:HD12	2.46	0.44
1:D:505:GLU:C	1:D:507:GLU:H	2.20	0.44
1:A:377:TRP:CH2	1:B:367:ILE:HG21	2.52	0.44
1:A:425:GLN:NE2	1:A:427:GLU:OE2	2.51	0.44
1:C:395:ASN:HD21	1:C:457:ARG:H	1.65	0.44
1:D:399:ARG:HA	1:D:402:SER:HB2	2.00	0.44
1:D:416:TRP:HB3	1:D:442:LEU:HD12	1.99	0.44
1:D:455:VAL:CG2	1:D:456:GLY:H	2.27	0.43
1:D:455:VAL:CG2	1:D:456:GLY:N	2.73	0.43
1:A:424:LEU:C	1:A:424:LEU:HD23	2.39	0.43
1:A:468:VAL:HA	1:A:478:LYS:O	2.19	0.42
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.88	0.42
1:C:435:GLU:HB2	1:C:442:LEU:HD23	2.01	0.42
1:D:390:SER:O	1:D:394:VAL:HG23	2.19	0.42
1:C:398:ILE:CG2	1:C:464:ASP:HB3	2.50	0.42
1:C:451:ARG:NH1	2:C:2:PO4:O4	2.53	0.42
1:C:390:SER:OG	1:C:391:SER:N	2.52	0.42
1:C:473:LEU:H	1:C:473:LEU:HG	1.71	0.42
1:A:420:LYS:HB3	1:A:421:ASP:H	1.79	0.41
1:B:451:ARG:HH11	1:B:451:ARG:HG3	1.86	0.41
1:A:429:GLU:CG	1:A:502:ILE:HD11	2.51	0.41
1:B:380:MET:O	1:B:477:LEU:HB2	2.21	0.41
1:C:451:ARG:HA	1:C:451:ARG:HD2	1.93	0.41
1:B:437:GLN:NE2	1:B:438:SER:H	2.18	0.41
1:D:468:VAL:HG22	1:D:479:CYS:HB2	2.03	0.41
1:A:464:ASP:OD1	1:A:464:ASP:N	2.53	0.41
1:C:425:GLN:HB2	1:C:432:LYS:HB2	2.03	0.41
1:A:382:GLU:CD	1:A:451:ARG:HH22	2.23	0.41
1:D:474:THR:OG1	1:D:476:MET:HG2	2.21	0.41
1:A:404:HIS:CD2	1:A:460:GLY:HA3	2.55	0.41
1:C:401:LEU:O	1:D:486:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:SER:HB3	1:B:417:GLY:O	2.21	0.40
1:A:368:LYS:HD2	1:A:494:SER:HB3	2.03	0.40
1:D:393:ALA:HA	1:D:396:ASN:HB2	2.03	0.40
1:B:432:LYS:O	1:B:433:LEU:HD23	2.21	0.40
1:A:378:VAL:HG23	1:A:401:LEU:HD11	2.03	0.40
1:C:433:LEU:O	1:C:442:LEU:HB2	2.21	0.40
1:B:377:TRP:C	1:B:377:TRP:CE3	2.95	0.40
1:D:396:ASN:O	1:D:400:GLN:HB2	2.22	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	123/148 (83%)	108 (88%)	14 (11%)	1 (1%)	27	58
1	B	120/148 (81%)	103 (86%)	14 (12%)	3 (2%)	9	21
1	C	123/148 (83%)	102 (83%)	20 (16%)	1 (1%)	27	58
1	D	119/148 (80%)	97 (82%)	19 (16%)	3 (2%)	9	21
All	All	485/592 (82%)	410 (84%)	67 (14%)	8 (2%)	14	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	B	506	LEU
1	D	488	ALA
1	B	441	LEU
1	D	455	VAL
1	B	474	THR
1	D	448	ILE
1	C	436	PRO

### 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	110/127 (87%)	102 (93%)	8 (7%)	20	44
1	B	107/127 (84%)	98 (92%)	9 (8%)	16	34
1	C	110/127 (87%)	97 (88%)	13 (12%)	8	18
1	D	106/127 (84%)	91 (86%)	15 (14%)	5	12
All	All	433/508 (85%)	388 (90%)	45 (10%)	10	23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	GLU
1	A	389	ARG
1	A	390	SER
1	A	448	ILE
1	A	452	VAL
1	A	457	ARG
1	A	458	ASP
1	A	464	ASP
1	B	367	ILE
1	B	385	LEU
1	B	402	SER
1	B	422	LEU
1	B	437	GLN
1	B	442	LEU
1	B	448	ILE
1	B	473	LEU
1	B	496	HIS
1	C	368	LYS
1	C	390	SER
1	C	392	VAL
1	C	395	ASN
1	C	402	SER
1	C	437	GLN
1	C	442	LEU
1	C	448	ILE
1	C	461	ARG

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Mol	Chain	Res	Type
1	C	462	GLU
1	C	473	LEU
1	C	489	LYS
1	C	507	GLU
1	D	368	LYS
1	D	396	ASN
1	D	433	LEU
1	D	437	GLN
1	D	442	LEU
1	D	452	VAL
1	D	462	GLU
1	D	463	ARG
1	D	464	ASP
1	D	474	THR
1	D	496	HIS
1	D	497	GLU
1	D	501	LYS
1	D	505	GLU
1	D	507	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	C	437	GLN
1	D	437	GLN
1	D	445	GLN
1	D	490	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	1	-	4,4,4	0.23	0	6,6,6	0.31	0
2	PO4	C	2	-	4,4,4	0.29	0	6,6,6	0.31	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	PO4	A	1	-	-	0/0/0/0	0/0/0/0
2	PO4	C	2	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	127/148 (85%)	0.16	2 (1%) 68 74	41, 60, 77, 85	0
1	B	126/148 (85%)	0.07	2 (1%) 68 74	38, 60, 80, 83	0
1	C	127/148 (85%)	0.03	3 (2%) 56 62	37, 57, 76, 79	0
1	D	125/148 (84%)	-0.05	0 100 100	38, 58, 79, 85	0
All	All	505/592 (85%)	0.05	7 (1%) 72 77	37, 59, 78, 85	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	GLY	6.3
1	A	367	ILE	4.1
1	C	367	ILE	3.5
1	C	366	GLY	3.4
1	C	420	LYS	2.1
1	B	505	GLU	2.1
1	B	378	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	C	2	5/5	0.13	-0.78	89,89,89,90	0
2	PO4	A	1	5/5	0.11	-1.84	83,84,84,84	0

## 6.5 Other polymers

There are no such residues in this entry.